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Reactivity Controlled Compression Ignition (RCCI) Combustion Using Methanol and Diesel in a Single Cylinder Research Engine

School of Engineering

Thesis submitted for examination for the degree of Master of Science in Technology.

Espoo 30.6.2018

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ABSTRACT OF THE
MASTER'S THESIS

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Date: 30.6.2018 Language: English Number of pages: 7+59

Department of Mechanical Engineering

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Conventional internal combustion engines have severe CO_2, NOx and particulate matter (PM) emission problems so that the majority of countries in the world have issued regulations to control the emission. Alternative fuels such as natural gas, methane and ethanol are studied to tackle the problem. Methanol also has the potential to reduce CO_2, NOx and PM emissions due to lower C/H ratio, local oxygen and high evaporation latent heat. Therefore, methanol, as a fuel, applied with advanced combustion technology provides possibilities to solve emission problems.

RCCI technology is discovered as an advanced engine technology to reduce NOx emissions as well as fossil fuel utilisation in the future. In the thesis, methanol and diesel are chosen to conduct the RCCI combustion. To reach the RCCI combustion mode, the diesel injection strategy is firstly tested, and the experiment is divided into two groups based on the diesel injection strategy: split diesel injection and single diesel injection. Within each group, methanol injection timing, methanol substitution rate (MSR), air mass flow and air intake temperature are the main parameters.

The results demonstrate the diesel injection strategy has a direct influence on the combustion characters. RCCI combustion mode can be reached in single and early diesel injection conditions, while the feature of combustion in split diesel injection condition is dominant by the pilot diesel fuel showing dual fuel or diesel combustion characters. Single diesel injection also reduces the NOx emissions. In both experiment groups, air intake temperature significantly active the fuel. Besides, in the single diesel injection group, each particular MSR has a precise and narrow diesel injection operation window.

Keywords: methanol, RCCI, reactivity stratification, injection strategy

Preface

The master thesis was conducted in the Internal Combustion Engine Laboratory, Aalto University. The thesis is funded by the European Union Project, Hercules2, and a minor funding granted by Henry Ford Foundation. I am grateful for all the organisations involved in the project providing research resources, facilities and financial support to complete the thesis.

I would like to express my sincere appreciation to my supervisor Professor Martti Larmi and Advisor D.Sc. (Tech) Ossi Kaario for all the knowledge and expertise they offered. I have learned plenty of knowledge not only about combustion science but also practical research skills.

I would also like to take this opportunity to thank research engineer Olli Ranta and Otto Blomstedt. Without their excellent technical support and patient instruction, I cannot finish the thesis experiment. Also, many thanks to my colleges Ari Ainsalo, Janak Aryal, Qiang Cheng and Zeeshan Ahamed who inspire me when I face problems. The working environment of the laboratory that provides pure academic atmosphere deserves all my respects.

Finally, all the words cannot express my great appreciation to my family and close friends for consistently supporting me during my study period in Europe. A particular honour belongs to my parents for all the understanding and support in my entire life.

Otaniemi, June 2018

Yabin Dong

Contents

Nomenclature

Abbreviations

AFR	Air fuel ratio
AIT	Air intake temperature
AMF	Air mass flow
ASI	After start of injection
bioDME	Bio-Dimethyl ether
BTDC	Before top dead centre
CA5	Crank angle for 5% heat releases
CA50	Crank angle for 50% heat releases
CI	Compression ignition engine
DI	Direct injection
DICI	Direct injection compression ignition
DIT	Diesel injection timing
DSR	Diesel substitution ratio
EGR	Exhaust gas recirculating
EHVA	Electrohydraulic valve actuator
EISFC	Effective indicated specific fuel consumption
EV	Electric vehicle
FFV	Flexible fuel vehicle
HCCI	Homogeneous charge compression ignition
HRR	Heat release rate
HTHR	High temperature heat release
HVO	Hydrotrated vegetable oil
ITE	Indicate thermal efficiency
ktoe	Thousand tons of oil equivalent
LHV	Lower heating value
LTHR	Low temperature heat release
MIT	Methanol injection timing
MSR	Methanol substitution ratio
NG	Natural gas
NTC	Negative temperature coefficient
PAH	Polycyclic aromatic hydrocarbons
PFI	Port fuel injection
PM	Particulate matter
PRF	Primary reference fuel
QHR	Cumulative heat release
RCCI	Reactivity controlled compression ignition
RI	Ringing intensity
RON	Research octane number
SCR	Selective catalytic reduction
SI	Spark ignition
TDC	Top dead centre

Symbols

λ	Lambda
ϕ	Equivalent ratio
C_{vff}	Coefficient of methanol vaporisation
$L_{gasoline}$	Latent heat of gasoline vaporisation
$L_{methanol}$	Latent heat of methanol vaporisation
γ	Ratio of specific heat
θ	Crank angle
$\dot{m}_f$	Fuel mass flow
$\dot{E}$	Energy flow
°C	Degree Celsius

Chemical Compounds

CH_3OH	Methanol
CH_3CH_2OH	Ethanol
CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
H_2	Hydrogen
H_2O	Water
NO	Nitric oxide
NO_2	Nitrogen oxide
NOx	Nitrogen oxides
O_2	Oxygen
SOx	Sulphur oxides

1 Introduction

Environment issues including air pollution, water pollution, fossil fuels utilisation and waste of natural resources are threatening the ecological environment of the earth. Energy-related activities have concerned the public because they generate a considerable amount of CO_2, SOx, NOx and particulate matters (PM). Energy system can be divided into four sectors: industry, resident, transportation and other service sectors. Due to the high energy intensity, transportation energy utilisation has attracted researchers attention. Most importantly, diesel, gasoline and other oil products accounted for 92% of total energy consumption in transport sector [1]. Therefore, advanced technologies must be implemented in the transportation sector to reduce oil products consumption and carbon emissions.

Using alternative fuels such as bio-diesel, hydrotreated vegetable oil (HVO), bio-dimethyl ether (bioDME), ethanol (CH_3CH_2OH) and methanol (CH_3OH) can be a solution to mitigate CO_2 emissions. Bio-diesel is derived from biomass and it can play an essential role in futures' carbon-neutral energy system; HVO, as a drop-in fuel, is regarded as the most prospective alternative fuel and has already dominated the renewable fuel market in Finland; BioDME also attracts people's attention, and the Volvo group has developed bioDME trucks [2]; Besides, E85 which contains 85% ethanol and 15% gasoline is widely used in flexible fuel vehicles (FFV). Due to similar properties to ethanol, methanol also has promising prospects as a fuel. However, all the alternative fuels are not the same as diesel or gasoline regarding physical and chemical properties, which brings limitations when using renewable fuels. Therefore, multiple solutions are needed to tackle problems in the transport sector.

Advanced power and combustion technologies also provide alternative approaches to reduce emissions. Electric vehicles (EV) can effectively reduce CO_2, NOx, SOx and particulate matters at the local level. The market share of EV has been rising significantly in recent years. However, EV cannot adapt to heavy load off-road conditions where internal combustion engine still dominates. Internal combustion engines are still widely used in the marine sector and the agricultural sector, but emission problems must be diminished. Dual fuel combustion technology uses two fuels in the one engine which reduces soot and NOx emissions. Besides, an advanced internal combustion engine technology, homogeneous charge compression ignition (HCCI) is developed. HCCI is a low temperature combustion technology combining the characters of compression ignition engines (CI) and spark ignition engines (SI). According to experiments, it achieves extremely low NOx emission [26]. Reactivity controlled compression ignition combustion (RCCI) is a modified technology based on HCCI technology, which uses two reactivity level fuels and improves the controllability of combustion phase in HCCI [30]. RCCI significantly strengthens engine combustion performance in terms of NOx emissions and thermal efficiency. It is also flexible to select fuels such as gasoline/diesel, Alkane/diesel and alcohol/diesel. However, more precise injection time control, the ratio of two fuel and other aspects need to be explored.

This thesis focuses on RCCI combustion using methanol and diesel in a single cylinder research engine LEO1. The majority research method is the LEO1 experiment, and it is supported by a GT-SUITE simulation. In the first stage, GT-SUITE is used to model the methanol evaporation and how it affects in-cylinder temperature. In the second stage, methanol/diesel are tested on LEO1 research engine. The methanol injection concept is port injection into the intake manifold. Methanol injection event is during the air intake stroke to create the homogeneous mixture, while diesel is injected around 20 to 50 degrees before top dead centre (TDC) depending on different combustion conditions. The air mass flow, air intake temperature, the substitution of energy from methanol, methanol injection timing, diesel injection events and diesel injection timing are studied.

The primary goals of this thesis are:

- Understand the principle and current research status of RCCI technology
- Study the properties of methanol and how methanol vaporisation affects in-cylinder temperature by GT-SUITE simulation
- Study the influence of multiple parameters on the RCCI combustion through LEO1 experiment. Specifically, study the influence of air mass flow (or ϕ) and air intake temperature on the RCCI combustion; study the methanol substitution rate and methanol injection timing influence on the methanol/diesel RCCI combustion; investigate diesel injection strategy, diesel injection timing impacts to the RCCI combustion; Study NOx emissions
- Understand the RCCI combustion characters and suggest promising working conditions for methanol/diesel RCCI combustion in middle load high speed engines

2 Background

2.1 Methanol

Methanol draws researchers' attention in recent years owing to its combustion properties and low emission characters. It has good prospects to be a main fuel for vehicles. Methanol is the simplest alcohol, and it is light, colourless, with alcohol odour and flammable. Besides, it should be noticed that methanol is highly toxic: only ten mL would cause permanent blindness [5]. In 2015, global demand for methanol was 70 million metric tons in all industries. Over 90 methanol plants distribute in all over the world with 110 million metric tons capacity to meet the considerable amount of methanol demand [6].

The corrosion properties of methanol should be noticed because it affects the materials choice of related equipment. Specifically, methanol is significantly corrosive to aluminium, and there are two mechanisms for aluminium corrosion. Firstly, methanol can react with aluminium oxide (Al_2O_3) which usually acts as the coating to protect aluminium. Secondly, methanol can oxidise aluminium directly. The two reactions are shown in reaction (a) and (b), respectively.

$$2CH_3OH + Al_2O_3 \rightarrow 2Al(OCH_3)_3 + 3H_2O \qquad (a)$$
$$CH_3OH + 3Al \rightarrow 2Al(OCH_3)_3 + 3H_2 \qquad (b)$$

During the thesis experiment, the methanol injector was plugged after three weeks. The main metal material of equipment is stainless steel, but the fuel filter is made from aluminium. The possible reason is that corroded metal residues block the methanol injector.

The widely used method to produce methanol is synthesis via syngas (CO_2 and H_2), and it has three processes: synthesis gas preparation, methanol synthesis and methanol purification [7]. Syngas can be produced from fossil resources such as natural gas and coal. Steam reforming (Reaction (c) and water gas shift (Reaction (d)) are the primary chemical reactions to produce syngas from natural gas. Other than steam reforming, partial oxidation and dry reforming are different approaches to produce natural gas derived syngas [8]. Besides, coal is another vital resource to general synthesis gas that contains partial oxidation (Reaction (e)) and water gas shift reaction (Reaction (d)). This process is also known as coal gasification. In addition, biomass, as a renewable raw material, is utilised to produce methanol as well, and similar to coal, gasification approach is mainly used in industrial level biomass for syngas conversion. The challenge in biomass to syngas conversion is the tar content, but usually, it can be tackled by choosing appropriate operating parameters for certain biomass. Although biomass derived synthesis still remains in small scale, it provides a sustainable approach to produce syngas and subsequently to methanol.

$$2CH_4 + 2H_2O \rightleftharpoons 2CO + 6H_2 \qquad (c)$$
$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad (d)$$

$$C + 1/2O_2 \rightleftharpoons CO_2 + H_2 \qquad \text{(e)}$$

The second step is the methanol synthesis including three chemical reactions. Reaction (h) is the reverse of water gas shift reaction and combine with Reaction (f) being the overall methanol synthesis Reaction (g). Finally, water, the main impurity is removed by heating up the liquid products [7].

$$CO + 2H_2 \rightleftharpoons CH_3OH \qquad \text{(f)}$$
$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \qquad \text{(g)}$$
$$CO_2 + H_2 \rightleftharpoons CO + H_2O \qquad \text{(h)}$$

Methanol is widely used in industries, especially in manufacturing other chemicals such as biodiesel, plastics, paints and textiles. It is a raw material for catalysed transesterification reacts to generate biodiesel (Reaction (i)), and it is a denaturing agent for ethanol that can be further used as a solvent [5],[9].

$$\text{Fatty acid}(R_1COOH) + \text{methanol} \rightleftharpoons \text{Ester}(R_1COOR) + H_2O \qquad \text{(i)}$$

Methanol is also an alternative fuel in internal combustion engines. The comparison among diesel, gasoline, ethanol and methanol are shown in Table 1. Each property is analysed in the following paragraphs.

Table 1: Fuel Properties Comparison [5],[10–14]

	Diesel	Gasoline	Methanol	Ethanol
Formula	C12-C20	C4-C12	CH_3OH	CH_3CH_2OH
Molecular Weight [g/mol]	150-250	60-150	32	46
Composition [%]				
Carbon	86.5	86.5	38	52
Hydrogen	13.5	13.5	12	13
Oxygen	0	0	50	35
C/H ratio	6.41	6.41	3.17	4
Cetane Number	min 51	—	3-5	11
Octane Number (RON)	—	min 95	108	109
Flash Point [°C]	55	40	11	17
auto-ignition Temperature [°C]	250	300	470	363
Flammability [Volume%]				
Lower limit	0.6	0.6	7	3.5
Higher limit	7.5	8	36	15
Stoichiometric AFR	14.5	14.7	6.4	8.9
LHV [MJ/kg]	43	42.7	20.27	26
Density at 15°C [kg/m^3]	820-845	720-775	790	790
Viscosity at 25°C [mPa.s]	3.35	0.5-0.6	0.544	1.074
Heat of Vaporisation [kJ/kg]	225-280	275-365	1155	904

Gasoline and diesel are refined from crude oil and both of them have complex chemical structures. Usually, gasoline is a mixture of alkanes, cycloalkanes and alkenes with four to twelve carbon atoms in each molecule. While diesel molecule is heavier,

with twelve to twenty carbon atoms in single diesel molecule, and it is mixed by saturated hydrocarbons such as alkane and aromatic hydrocarbons, alkylbenzenes. Fig.1 indicates the chemical structure of basic hydrocarbons. In the fuel combustion process, the long chain molecule of gasoline and diesel is firstly cracked into small alkanes and other hydrocarbons. Then the simple radicals are further converted to CO_2 and H_2O.

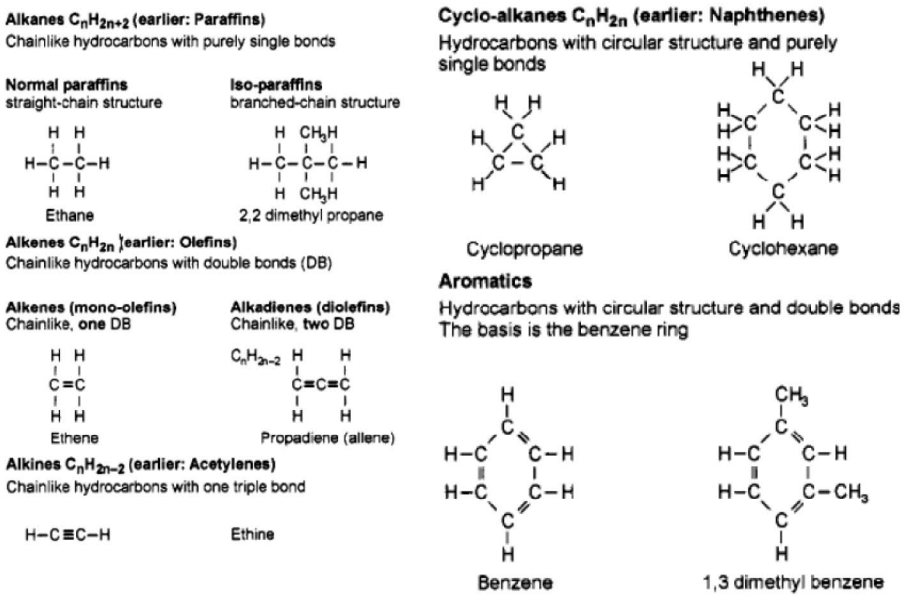


Figure 1: Chemical Structure of Alkane, Alkene, Alkine and Aromatics [15]

Methanol and ethanol are in the alcohol group with the common formula, R-OH, in which a hydrogen atom is replaced by a -OH radical to connect with carbon atoms. Fig. 2 illustrates the chemical structure of methanol and ethanol.

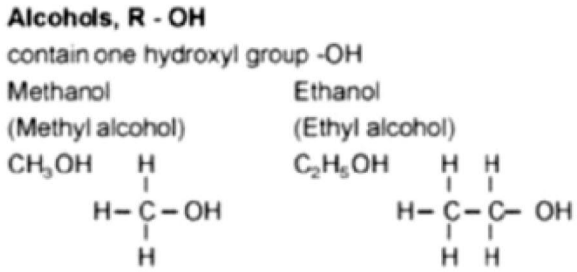


Figure 2: Chemical Structure of Methanol and Ethanol [15]

The composition difference between alcohol and fossil fuel brings significant different combustion behaviours. As listed in Table 1, the C/H ratio of diesel and gasoline

is around 6.41, while the C/H ratio for methanol and ethanol are 3.17 and 4, respectively. C/H ratio acts as an effective emission indicator, and a higher C/H ratio means higher CO_2 emissions. The C/H ratio of methanol is around fifty percent lower than that of diesel and therefore, methanol does benefit the environment from carbon emission's point of view. Besides, the oxygen content of alcohol fuel can reduce PM emissions, since local oxygen provides sufficient oxidiser. While, the slightly higher NOx emission is observed with the present of oxygen [16].

Cetane number reflects the ignition properties of CI fuel, and higher cetane number indicates the fuel is easier to be compression ignited. There are two references to determine the cetane number of a certain fuel, n-hexadecane ($C_{16}H_{34}$) with cetane number 100 and α-methyl naphthalene ($C_{11}H_{10}$) with cetane number 0 [15]. According to the European standard, the minimum cetane number of diesel fuel is 51. By contrast, the cetane number of methanol is less than 5, which brings the challenge of compression ignition. Octane number indicates the knocking resistance of SI fuels. Similar to cetane number, the octane number of a fuel refers to ISO-octane (C_8H_{18}) that octane number is 100 and n-heptane (C_7H_{16}) that octane number is 0. Knocking is a phenomenon that combustion of the fuel occurs before flame front reach that location. It causes the unbalanced pressure distribution in the cylinder that is harmful to the engine. The octane number of methanol is 108, so it has desired knocking resistance.

Auto-ignition temperature is also a crucial property of CI fuel due to the ignition principle of the diesel engine. Unlike SI engine which has a spark plug to ignite the fuel, the ignition of CI engine is depended on the in-cylinder pressure and temperature. The auto-ignition temperature of methanol is 470°C, but diesel can burn without ignitions resources when the temperature reaches 250°C. It brings the challenge to ignite the methanol and usually a higher compression ratio or ignite improver are used to tackle the problem.

LHV indicates the energy content of the fuel. It is clear that both diesel and gasoline have much high energy content than alcohol fuels (Table 1). It means producing the same amount of power, much more alcohol fuels are needed if the efficiency is the same. Besides, it should notice that the latent heat of methanol vaporisation is significantly higher than that of diesel. The fuels have to evaporate to the gas phase to be burned, and inevitably the methanol evaporation brings strong cooling effects to the cylinder leading to cylinder peak pressure drop. The cooling effect of methanol vaporisation makes methanol ignition even more difficult. In the thesis, methanol cooling effect is modelled in GT-SUITE and the results are shown in chapter 4. However, the benefit of methanol cooling effect is that the low temperature can result in low NOx emissions. Also, the cooling process increases the engine efficiency, since the engine components are cooling down and it reduces heat losses [13].

To summarise, methanol benefits the combustion because it reduces the emissions; however, the ignition difficulty and lower energy content negatively affect the com-

bustion. Therefore, the utilisation of methanol as a fuel needs to be further explored.

2.2 Methanol Application in Transport Sector

Methanol has received more attention as an alternative fuel in both automotive industry and marine industry. According to EN 228 standard, the limitation of the oxygen content of the transport fuel is 2.7% (m/m) corresponding to 5.4% (m/m) methanol. Additionally, EN 228 specified only 3% (V/V) methanol can be added and stabilising agents is needed. For light-duty vehicles, a low percentage of methanol can be blended with gasoline in the conventional SI engines. The application of methanol in heavy-duty vehicles such as trucks is still being researched. Regarding marine application, methanol is a promising and safe alternative fuel in ships to reduce NOx, SOx and PM. MAN Group and Wärtsilä have already developed dual fuel marine engines using methanol.

One desirable methanol application in the automotive industry is methanol fuel cell. The Danish company, SerEnergy has developed the methanol fuel cell vehicle with the range up to 800 km within one tank methanol. SerEnergy developed the first generation Reformed Methanol Fuel Cell (RMFC) on Fiat 500 platform, and the latest RMFC is based on Nissan e-NV200. The Nissan e-NV200 RMFC vehicle enables up to 800 km which can satisfy the utilisation such as urban taxis and delivery van [17].

To understand the potential of methanol in the marine sector, a methanol market investigation and application research, Sustainable Marine Methanol (SUMMETH), has been conducting in Sweden and Finland, carried on by SSPA Sweden, ScandiNAOS, Lund University, VTT Technical Research Centre of Finland etc. The project attempts to investigate methanol market in Nordic countries and to develop advanced methanol engines. Based on their study of DICI Diesel engine, DICI Diesel engine with SCR, PFI-SI Lean Burn engine, etc., they conclude methanol can have a promising future, but the modification of engines is inevitable. More specific, despite most of the current methanol engines are robust, none of the engine models is as rugged as diesel engines. Particularly, in-cylinder corrosion is revealed in the premixed engine types such as PFI-SI engine, if the engine is not warming up properly [18].

While most of the current methanol engines are amended from HFO/diesel/gas dual-fuel engines, a few numbers of engines are available for methanol retrofit. Specifically, fuel tanks, piping and bunker systems need to be modified. For instance, boilers and fuel separators are necessary for HFO-engine ships, but they are not required when methanol is the primary fuel. MAN Group and Wärtsilä developed methanol retrofit solutions for marine engines that are under operation.

In 2016, seven ocean vessels equipped with B&W ME-LGI 2-stroke dual fuel engine start operating. The engine is developed by MAN Group and it can run by methanol, fuel oil, marine diesel oil or gas oil. Fig.3 shows the overview of the ME-LGI engine

system which contains Fuel valve train (GVU), Methanol supply system, Methanol Cargo fuel pump and methanol service tank. The ME-LGI engine uses temperature-conditioned methanol at constant supply pressure, and the fuel flow rate is adjusted depending on the engine load. Methanol valve train connects the fuel supply system with the ME-LGI engine through a master fuel valve. The combustion chamber is also designed to cope with the corrosive environment.

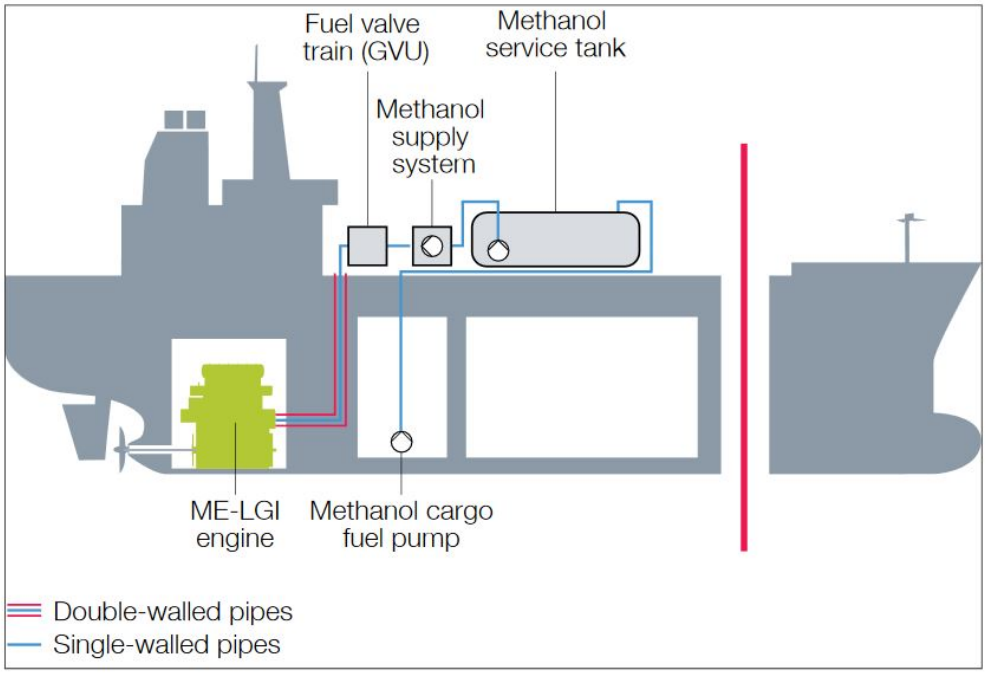


Figure 3: ME-LGI Engine and Engine Auxiliary System Overview [20]

Wärtsilä also develops Gas-Diesel engines which can run by gas and liquid fuels. In the Wärtsilä methanol-diesel retrofit solution, methanol is ignited by the pilot diesel fuel. Compared with the conventional diesel engine, methanol common rail system is added to the engine. The Cylinder head is modified for dual fuel inlet, methanol pump, sealing and control oil are updated for methanol application. Emission tests have been conducted on Wärtsilä Sulzer ZA40S-MD methanol-diesel engine and the results are promising for clean operation. NOx emission is 3-5 g/kWh which meets the Low Tier II demand, both CO and unburned HC are less than 1 g/kWh [19].

2.3 Combustion

Combustion converts the chemical energy of fuels to heat that can be used directly or further converted to mechanical energy to generate electricity. According to IEA, the world produced 24 million GWh of electricity and 13 million TJ heat in 2015 [1].

68% of power and 96% of heat is from coal, natural gas, oil and biomass which need to be burned to generate electricity and heat. Thus, combustion is still the majority approach to utilise energy.

Internal combustion engine outputs mechanical power by extracting energy in fuels via combustion reaction in the cylinders. Fuels are burned in the combustion chambers to generate high temperature and high pressure gas which delivers power to the piston. This process is done in the power stroke of a typical 4-stroke piston engine combining with air intake stroke, compression stroke and exhaust stroke to complete an engine cycle. Based on the principle of ignition, typical internal combustion engines are divided into compression ignition engine and spark ignition engine. The details of CI engine and SI engine are introduced in the following sections.

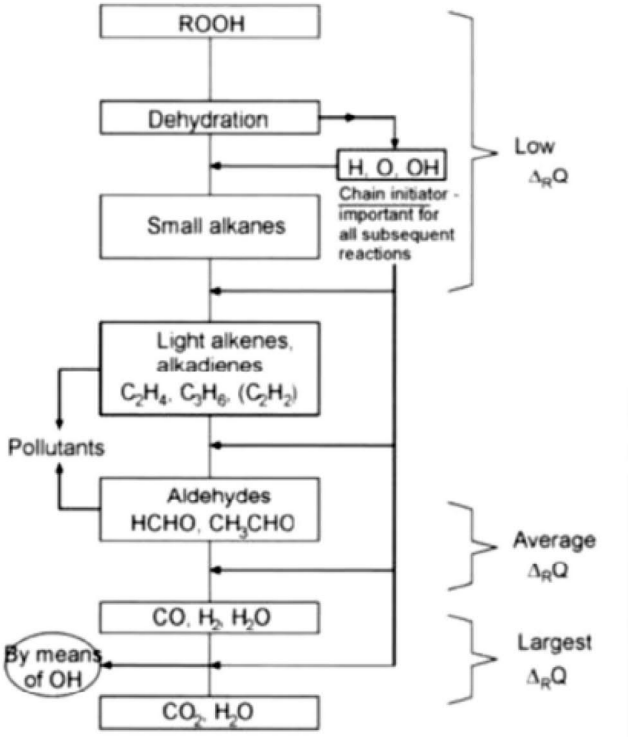


Figure 4: Hydrocarbon Oxidation Process [15]

The principle of diesel and gasoline combustion is the oxidation of hydrocarbons. Fig.4 illustrates the reaction stages: the first stage is to form aldehydes such as CH_3CHO and HCHO. To generate aldehydes, the hydrocarbon peroxides (ROOH) are broken down into small alkanes by dehydrogenation. Intermediate products react with produced -O, -H, -OH radicals to form alkenes and aldehydes, then finally generate aldehydes. Around 5% of heat is released in this stage, and the related crank angle is defined as the start of combustion (CA5) in the internal combustion engine industry; the second stage forms CO and H_2 with blue flame; CO_2 and part

of H_2O are ultimately generated in the final stage. Most heat is released in the third stage, which leads to the significant temperature rise.

Fig.5 illustrates the intermediate radicals concentrations over time and the tendency of temperature. It shows -H, -O and -OH radicals are generated in the early stage, and their concentration keeps high until CO_2 and H_2O occur. -OH radical plays an essential role in the optical engine research to identify the combustion stage. Besides, it is indicated in the Fig.5 the combustion stages contain alkane, alkene formation, aldehydes formation, CO, H_2 generation and finally CO_2 and H_2O producing. The temperature rises slightly in the first two combustion stages, while a sharp increasing occurs when H_2O and CO_2 start to generate.

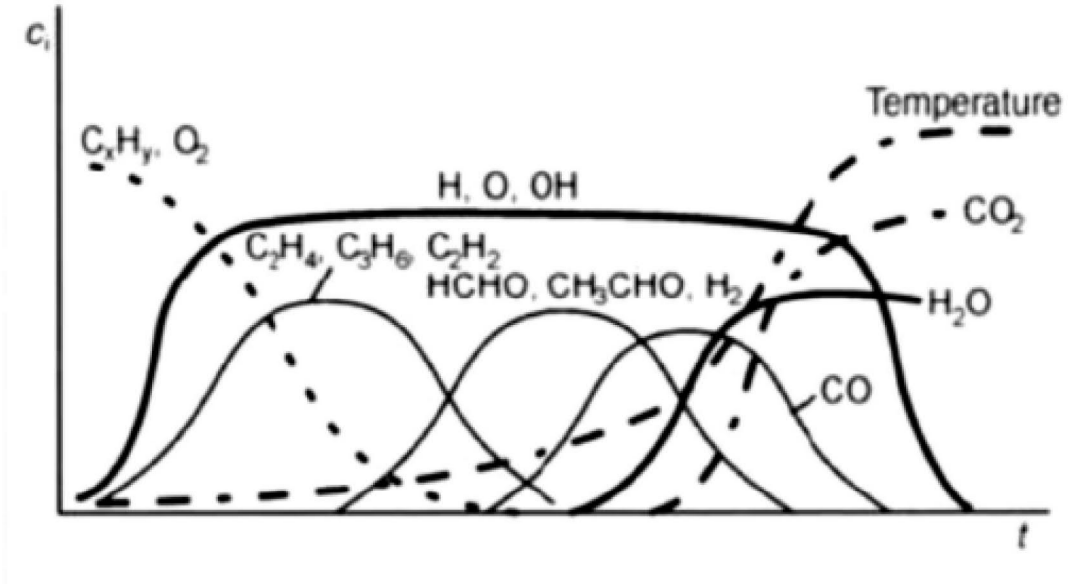


Figure 5: Combustion Temperature and Intermediate Products Concentration Over Time [15]

In the industry application, the combustion can be simplified as the reaction (j) [15]: hydrocarbon reacts with oxygen generating H_2O and CO_2 with heat release.

$$C_xH_y + (\mathrm{x} + \tfrac{y}{4})\ \mathrm{O_2} \rightarrow \mathrm{xCO_2} + \tfrac{y}{2}\ \mathrm{H_2O} + \Delta_R\mathrm{H} \quad \text{(j)}$$

When the fuel can be completely oxidised by the right amount of air to generate only carbon dioxide and water, the combustion condition is regarded as stoichiometric. The mass ratio between air and fuel is defined as air fuel ratio (AFR); λ is defined as actual AFR over stoichiometric AFR. Equivalent ratio ϕ ($\phi = 1/\lambda$), the reverse of λ, is also widely used. In the RCCI combustion concept, ϕ is more common and therefore, the thesis experiment uses ϕ to indicate the relation between air and fuel. As shown in Table 1, the AFR of diesel and gasoline is around 14.7. While due to the local oxygen, the AFR of methanol and ethanol are 6.4 and 8.9, respectively.

$$AFR = \frac{\dot{m}_{air}}{\dot{m}_{fuel}} \tag{1}$$

$$\lambda = \frac{AFR_{real}}{AFR_{stoichiometric}} \tag{2}$$

λ has strong influences on the internal combustion engines, especially on soot and NOx formation. λ greater than 1 is the lean condition while λ smaller than 1 is the rich condition. In diesel engine, soot is likely to form in very rich conditions, while NOx generates in relatively lean conditions. However, in terms of NOx formation, despite λ affects NOx generation, the NOx is the most sensitive to temperature. In general, diesel engine works in lean conditions and λ can even reach 5. Gasoline engine, as a premixed combustion engine, works in around stoichiometric conditions. However, considering the efficiency of three-way catalyst for exhaust gas treatment, SI engines usually operate under slight lean conditions.

2.3.1 Premixed Combustion

In premixed combustion mode, air and fuel are mixed in advance to create homogeneous conditions before ignition. Theoretically, premixed combustion presents stoichiometric (λ=1) air-fuel ratio conditions. In practical, lambda is slightly below or over 1 depending on operation conditions. Premixed combustion is inherently exothermic radical reactions, and once ignited, the combustion can be self-maintained by the released heat. The premixed combustion starts from the ignitions source and it develops via flame front propagation. The chemical reactions occur at the flame front and it separates burned and unburned fuels. The speed of flame front propagation is known as flame speed which is dependent on the reaction environment and reaction rate of reactants [21]. It reflects the speed of flame development, and usually, a laminar flame has the velocity between 0.5-2 m/s. Due to the movement of engine, laminar flame barely occurs in the internal combustion engines. While turbulent premixed flame is usually happening in the engines, which can reach the velocity of 20-25 m/s [22]. Turbulent premixed combustion is related to the many variables such as swirl, temperature and density.

The combustion in gasoline engines is premixed turbulent combustion. The fuel and air mixture is ignited at stoichiometric conditions by the spark plug followed by the flame front propagation, and it extinguishes when reaches the wall. Gasoline engine has intake, compression, combustion and exhaust strokes. The fuel is injected into the intake manifold with air or directly injected (DI) into the cylinder in the intake stroke. At the end of compression stroke, the spark plug ignites fuel-air mixture and deliver power in the power stroke

Knocking is one of the abnormal combustion phenomenon related to SI engines. If the temperature and pressure of the end gas exceed the auto-ignition limitations,

the remaining fuel in the end gas will burn before the flame propagation reaches the location [21]. This phenomenon is regarded as engine knocking. It leads to local pressure and temperature rising, which resulting in in-cylinder pressure fluctuating. The slight knock leads to noises of engines and severe knock can damage the engine components.

There are mainly two knocking mechanisms, spark-knock and knock caused by surface ignition. Spark-knock is defined as the auto-ignition repeatedly occurs, which means it varies cycle to cycle in cylinders and spark-knock can occur at different locations out of the flame region. Fig.6 illustrates normal cylinder pressure and knocking cylinder pressure. It is clear that due to the pressure waves caused by knocking, the in-cylinder pressure is not a smooth curve. Spark-knock can be controlled by retarding the spark timing or reducing the engine load. In Fig.6, By retarding the sparking timing from 32° BTDC to 28° BTDC, the knocking is significantly weakened. Distinguished from spark-knock, surface ignition is caused by the hot spot (deposit such as soot) on the wall of the cylinder, plug or valve. It can occur before the spark or after the spark. Thus, when the auto-ignition caused by hot surface happens out of the flame region, knocking occurs. The surface ignition caused knocking cannot be avoided by delay the spark timing, because the spark source is not the reason for knocking in such situations. Instead, it can be eliminated by changing the mechanical design of engines [21],[22]. The surface ignition has more rapid temperature and pressure rise, so knocking is more likely induced by the hot surface.

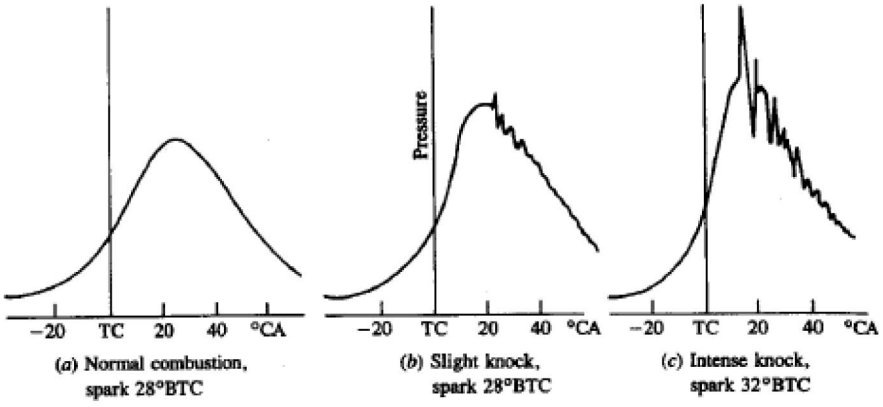


Figure 6: Comparison Among Normal Cylinder Pressure and Knocking Cylinder Pressure [21]

2.3.2 Non-premixed Combustion

Different from premixed combustion, the fuel and air are not mixed before ignition in non-premixed combustion. Diffusion flame is going to describe the flame character of non-premixed combustion. Diffusion flame speed is limited by the diffusion

rate which includes fuel penetration, evaporation and mixing with air. Therefore, diffusion flame is slower than premixed flame.

The diesel fuel continuously mixes with air after injected into the combustion chamber. The mixing process occurs at the surface of diesel jet where the combustion is premixed combustion. Diesel combustion tends to generate more soot because the centre of the fuel region has low local λ resulting in incomplete combustion. Owing to the high temperature, the soot becomes incandescent and radiates visible yellow light. Besides, more NOx is formed due to the high combustion temperature. Thus, because of this characters, diesel combustion causes serious environmental problems.

In diesel engine, the fuel is injected at the end of compression stroke close to TDC when the temperature and pressure reach the auto-ignition conditions of diesel. Due to the ignition principle, diesel engine is also named as compression ignition engine. Since the diesel is injected close to the TDC, there is no risk of knocking in standard diesel engines. Hence, the diesel engine can reach higher compression ratio leading to higher efficiency. However, as mentioned before, high combustion temperature brings severe NOx and soot emission problems in diesel engine. Principally, combustion in diesel engine is divided into four main phases: ignition delay, premixed combustion, diffusion combustion and late combustion.

Ignition delay is an important indicator for diesel combustion. It is defined as the time interval between the start of fuel injection and the start of ignition [21]. The ignition delay is due to the physical and chemical changes: on the one hand, the liquid fuel experiences atomisation and vaporisation; on the other hand, as analysed in section 2.2, the chemical process starts with long diesel molecular absorbs heat and crank into short chains, which prepares for completed combustion.

Premixed combustion is following the ignition delay, and the in-cylinder temperature has reached the auto-ignition temperature of diesel at this moment. Premixed combustion occurs leading to rapid heat release. However, the premixed combustion phase only lasts an around 2-3 crank angles.

Diffusion combustion is known as mixing-controlled-burn [23] because this phase is controlled by the in-cylinder air and fuel mixing. According to John E. Dec's study [23], the soot concentration is becoming higher and the size of soot particles are larger in this phase. Besides, the fuel atomisation and evaporation process continue in this phase.

Late combustion phase occurs when temperature and oxygen concentration is low. It takes place at later expansion stroke with lower heat release rate. The heat release is from unburned fuel or soot burning in this process. As such, it has significant influences on the exhaust gas emissions.

John E. Dec [23] studied the diesel combustion mechanisms by laser-sheet imaging

and summarised a conceptual model of diesel combustion. Fig.7 illustrates diesel combustion process in detail. The initial jet fuel development occurs at 0-4.5° after the start of injection (ASI) when liquid fuel penetrates in the cylinder and evaporates to gas phase. Auto-ignition occurs between 3-5° ASI depending on different operating conditions. John E. Dec summarises that diesel molecular breaks down to short chain and polycyclic aromatic hydrocarbons (PAH) at 4.5-5° ASI. It is followed by small soot particles generation between 5-6° ASI. Diffusion flame first takes place at around 6.5° ASI and it can be observed from the figure the diffusion flame covers the whole portion of fuel at downstream. The jet fuel piece continuously penetrates in the cylinder and higher concentration soot formed at around 9° ASI. Mixing controlled combustion condition is reached between 9° ASI to the end of injection.

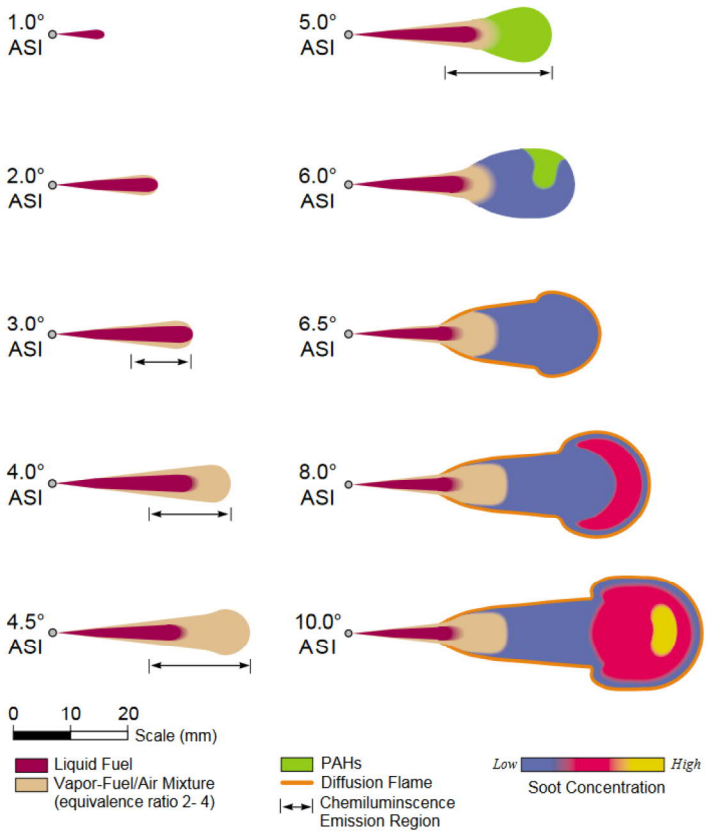


Figure 7: Scheme of Diesel Combustion Model [23]

2.3.3 Dual Fuel Combustion

Dual fuel combustion engine uses two types of fuels in which both premixed combustion, and non-premixed combustion exist. The low reactivity fuel (CH_4, NG, ethanol, methanol, etc.) is injected in the early stage to mix with air and it is ignited by the high reactivity fuel (usually diesel) which is injected close to TDC.

The small amount of diesel fuel, also known as pilot fuel, burns after injection and causes the in-cylinder temperature reaches the auto-ignition temperature of the premixed fuel. Then the premixed combustion occurs. The dual fuel concept is similar to RCCI combustion, but the principle is different due to the high reactivity fuel injection timing. The high reactivity fuel in dual fuel is injected close to TDC which means the dual fuel combustion depends on both high reactivity fuel spray physics and chemical kinetics of premixed fuel. By contrast, RCCI combustion is only relied on chemical kinetics because of earlier high reactivity fuel injection.

The heat release of dual fuel combustion can be divided into three overlapping phases [24]. Diffusion flame of pilot diesel is formed in the first stage that contains diesel fuel injection, evaporation and auto-ignition. When the surrounding temperature reaches the auto-ignition point of the premixed fuel, the second phase starts. The low reactivity fuel combustion is surrounding the diesel pilot premixed region. The last stage is the premixed turbulent flame propagation. Fig.8 illustrates three phases in both heavy load and light load conditions. Additionally, G. A. Karim [24] studied the influence of λ in dual fuel combustion. When dual fuel is operated at very lean conditions, the premixed fuel enters a rich and high temperature area. As a result, most premixed fuel is burned in the first and second phase, so there is no significant flame propagation in the last phase.

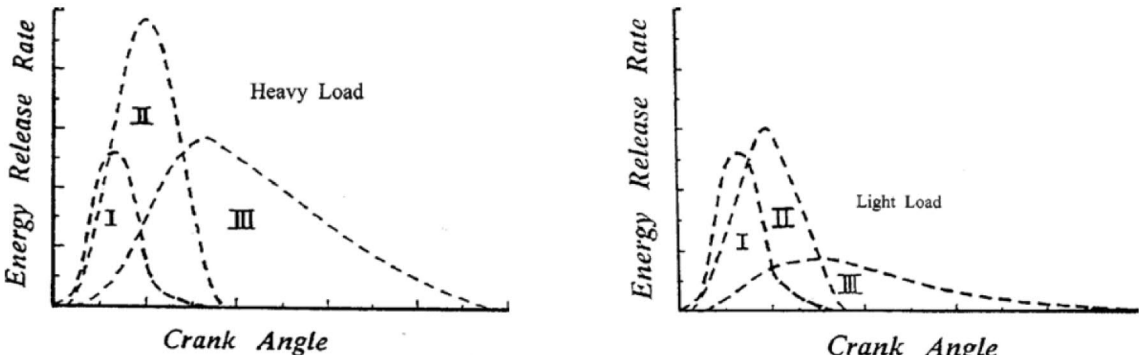


Figure 8: Dual Fuel Combustion Phase [24]

R. Pettinen studied the methane/diesel dual fuel combustion characters in high load lean conditions. The results suggest the rapid premixed flame propagation occurs when methane λ is lower than 2.2. Besides, it also concludes that to reach high efficiency, the methane substitution rate should be higher than 90% and overall λ be greater than 2 [22]. Z. Ahmad studied methane/diesel dual fuel via an optical engine, and the results indicate premixed flame fronts derive from combustion chamber wall propagating to the centre. Also, the ignition delay in 82% to 88% methane substitution is 1.5 to 2 times longer than diesel fuel combustion [25].

2.3.4 Homogeneous Charge Compression Ignition Combustion (HCCI)

Homogeneous charge compression ignition combustion (HCCI) combines the features of SI combustion, and CI combustion. The diesel is injected early and it is usually split into multiple times. The premixed air and fuel are compressed to reach the auto-ignition point, which ignites the fuel. HCCI combustion initiates at the different locations in the cylinder, so there is no identifiable flame front. Thus, HCCI combustion does not have local high temperature reaction zone [26], which significantly reduces NOx and PM emissions. Besides, unlike diesel combustion, the HCCI combustion is faster owing to the premixed diesel. However, due to premixed fuel, knocking of HCCI is a serious problem which limits its utilisation to lean air/fuel mixing conditions.

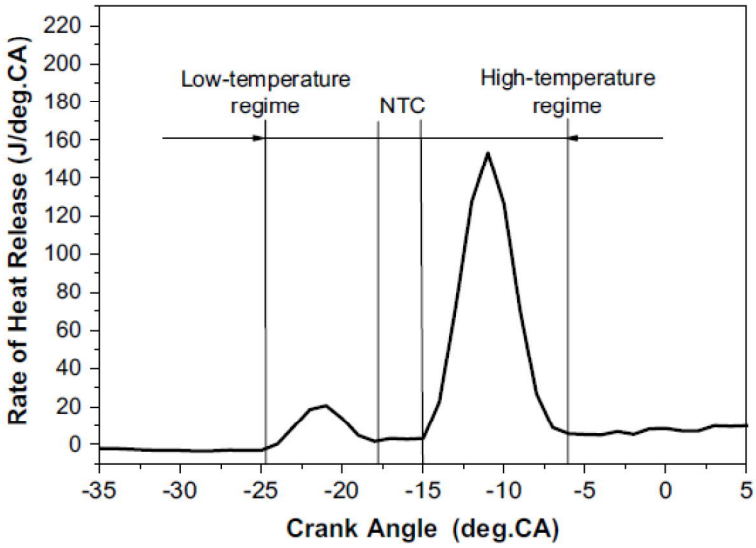


Figure 9: Typical HRR Curve for HCCI Combustion of N-Heptane Fuel [26]

R. Stanglmaier, C. Roberts, Furutani and Pucher studied the heat release characters of HCCI combustion and they conclude the three-stage heat release showing in Fig.9. It includes a low-temperature regime, negative temperature coefficient regime (NTC) and high-temperature regime. Fuel's octane number affects the low-temperature heat release which is associated with knocking in HCCI combustion. It is observed more significant low-temperature heat release occurs if the octane number of the fuel is low. In the NTC regime, the in-cylinder temperature increases and the overall HRR decreases. The global heat release is hence reducing. After that, the in-cylinder temperature reaches the auto-ignition point so that high temperature heat release occurs.

Chalmers University of Technology studied the feasibility of HCCI combustion of a passenger car [28]. The experiment reduces the compression ratio from 17:1 to 11.5:1 and uses high rate exhaust gas recirculating (EGR) to prevent knocking. The results

show the combustion phase is adequately controlled in lower compression ratio and high EGR rate, while the coefficient of variation (COV) is around 7% suggesting unstable combustion due to early ignition. Besides, the results suggest NOx and soot emissions are reduced by more than 95%, but the HC and CO emissions increased significantly. It indicates the incomplete fuel combustion in HCCI mode resulting in fuel consumption rising around 10-20%.

2.4 Reactivity Controlled Compression Ignition (RCCI)

Reactivity controlled compression ignition combustion is developed by the University of Wisconsin-Madison Engine Research Centre. It is a variation of HCCI combustion mode that a low reactivity fuel is applied with the high reactivity fuel to control the combustion. In general, high reactivity refers to the fuel with high cetane numbers such as diesel. On the contrary, gasoline, CH_4 and alcohol which have low cetane number are used as low reactivity fuels. Thus, the RCCI also belongs to dual fuel technology, but its combustion mechanism is similar to HCCI mode instead of conventional dual fuel mode. The motivation for developing RCCI technology is that it has high efficiency, low NOx and PM emissions due to the low combustion temperature. Besides, the low reactivity fuel makes it more feasible to control compared to HCCI mode. In the laboratory scale, the iso-octane/n-heptane, gasoline/diesel, Alkane/diesel and alcohol/diesel are widely studied. This master thesis will continue the previous study and focus on methanol/diesel to discover the RCCI combustion behaviours.

There are mainly two methanol injection strategies: port injection to the intake manifold and direct injection to the combustion chamber. Z.Q. Jia [29] studied the methanol injection strategy, and she concludes port injection and direct injection have similar patterns, but the thermal efficiency is slightly higher in the port injection case. Distinguished from dual fuel mode in which diesel injection timing is close to TDC, the diesel injection of RCCI mode is usually earlier than 15 CAD BTDC. Early diesel injection is to form a homogeneous mixture of methanol, diesel and air. As a result, the reactivity stratification is created leading to promising combustion mode. More specific, methanol has high octane number preventing the early combustion which occurs in high load HCCI mode. Besides, the low cetane number of methanol can be balanced by diesel fuel. The adverse cooling effect of methanol is diminished by increasing air intake temperature.

The typical HRR curve is shown in Fig.10, and it is similar to HCCI mode that two-stage of heat release occurs. J. Li et al. [31] reviewed the RCCI combustion characters and concluded identical behaviour to HCCI, that the low temperature heat release (LTHR) is governed by high reactivity fuel and NTC. High temperature heat release is controlled by the premixed fuel. RCCI research defines LTHR as the timing when $dQ/d\theta$ is greater than 0.5 [J/CAD] and HTHR is the timing when $dQ/d\theta$ exceeds 2 [J/CAD]. K. Inagaki studied the LTHR and HTHR behaviour of different octane number fuels and fuel substitution ratio. His research found the start

of LTHR is advanced with RON decreasing and a stronger LTHR peak occurs in lower RON case. Besides, the results also indicate the LTHR is reduced if more low RON fuel is used in the experiment. K. Inagaki's research illustrates the RCCI fuel heat release is significantly affected by the in-cylinder fuel reactivity stratification, namely, the properties of chosen fuels and mixing strategy [30].

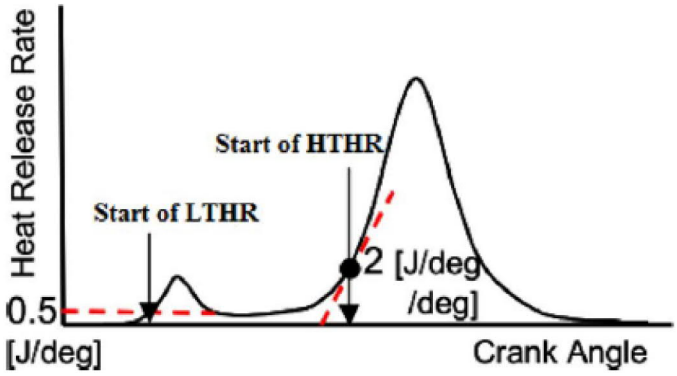


Figure 10: Typical HRR Curve for RCCI Combustion [30]

Besides of reactivity stratification, due to uneven mixing in the combustion chamber, the local λ is also different in the cylinder. The combustion at the local rich region will produce soot and NOx. Additionally, owing to fuel distribution in the combustion chamber, the fuel evaporation process will also lead to temperature stratification in the cylinder. Other parameters such as diesel injection strategy, EGR ratio, compression ratio and bowl geometry also influence RCCI combustion. The following section will analyse each parameter.

2.4.1 Influence of Parameters on RCCI

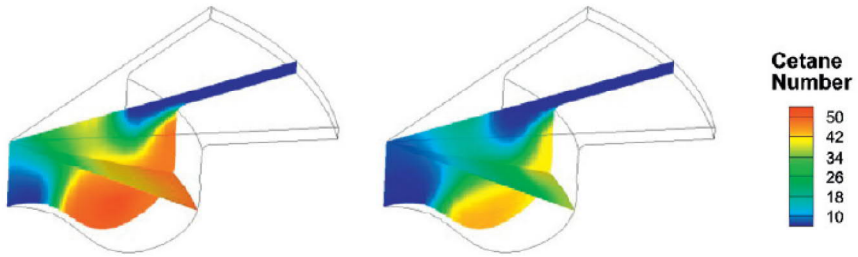
Fuel ratio: Methanol substitution rate (MSR) is typically used to measure the fuel ratio. It calculates from the energy content of two fuels (Eq.3), where $\dot{E}$ refers to the energy flow. According to the previous study, the low reactivity fuel ratio can even reach 90%. The fuel reactivity is eventually quantified by fuel cetane number which is decided by the methanol substitution rate. Eq.4 indicates the calculation of RCCI fuel cetane number, where X is the mole fraction of each fuel.

$$MSR = \frac{\dot{E}_{methanol}}{\dot{E}_{methanol} + \dot{E}_{diesel}} \tag{3}$$

$$CN_{RCCI} = \frac{CN_{diesel} \times X_{diesel} + CN_{methanol} \times X_{methanol}}{X_{diesel} + X_{methanol}} \quad [28] \tag{4}$$

Y.P. Li et al. studied methanol/diesel RCCI combustion by CFD simulation and concluded the combustion characters and emission behaviours [32]. The result shows

the ignition delay increases and the peak of HRR decreases with MSR increasing. The simulation results also suggest the CN distribution is not homogeneous in the combustion chamber and combustion phase stratification is observed (Fig.11). High CN region usually contains more diesel fuel and it is ignited first. Then the methanol with low CN is ignited by diesel. Y.P. Li concluded that with higher MSR, this combustion stratification is more significant. As a result, the heat release from the initial combustion phase is decreased due to the lower reaction rate, which further leads to HRR peak decreasing.



(a) Methanol mass fraction is 40% (b) Methanol mass fraction is 60%

Figure 11: Cetane Number Distribution in Different MSR at 4° BTDC. Port Methanol Injection; Diesel Injection Timing: 27° BTDC [32]

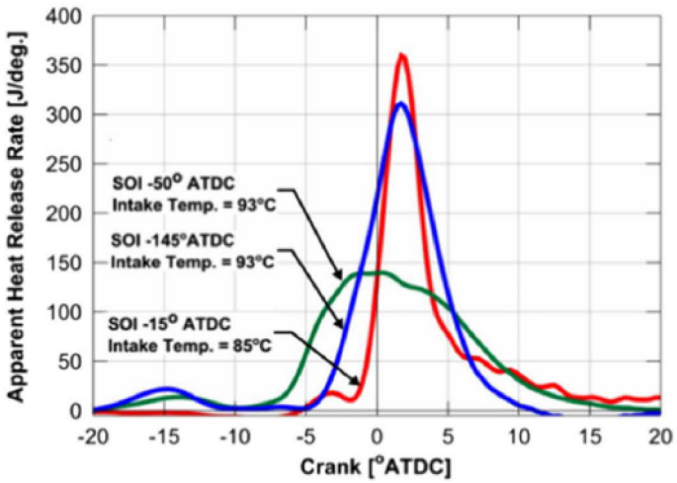


Figure 12: Apparent Heat Release Rates of RCCI [33]

Injection Strategy: The diesel injection strategy including main diesel injection timing and the number of diesel pulses has a significant influence on the RCCI combustion. S. Kokjohn further investigated the iso-octane/n-heptane fuel reactivity stratification in RCCI mode via high-speed chemiluminescence images and fuel

tracer fluorescence [33]. The research exams the fuel mixture at three different n-heptane injection timings: 145°, 50° and 15° BTDC. The results indicate the 145° BTDC and 15° BTDC cases have similar HRR curve, while the less heat is released in 50° BTDC case. As shown in Fig.12, the heat release duration of 50° BTDC is longer than 15° and 145° BTDC cases, but the peak of HRR is much lower. A tail can be observed from 15° BTDC case, and S. Kokjohn explains it as the slow combustion inside rich region of the n-heptane jet and some lean regions of iso-octane.

Single-shot images indicate the mixing conditions of three diesel injection timing illustrated in Fig.13. PRF number is defined as the iso-octane mass fraction in the charge. It is observed that the mixing conditions of iso-octane and n-heptane are quite homogeneous in the 145° BTDC case. In 15° BTDC case, although there is no sufficient time for iso-octane and n-heptane to mix, violent combustion occurs in the early part resulting in high heat release. The fuel reactivity shows linear like behaviour in 50° BTDC case, and the reactivity level decreases closer to the centre. Thus, it can be concluded the diesel injection timing affects fuel mixture and subsequently, it leads to different combustion mechanisms.

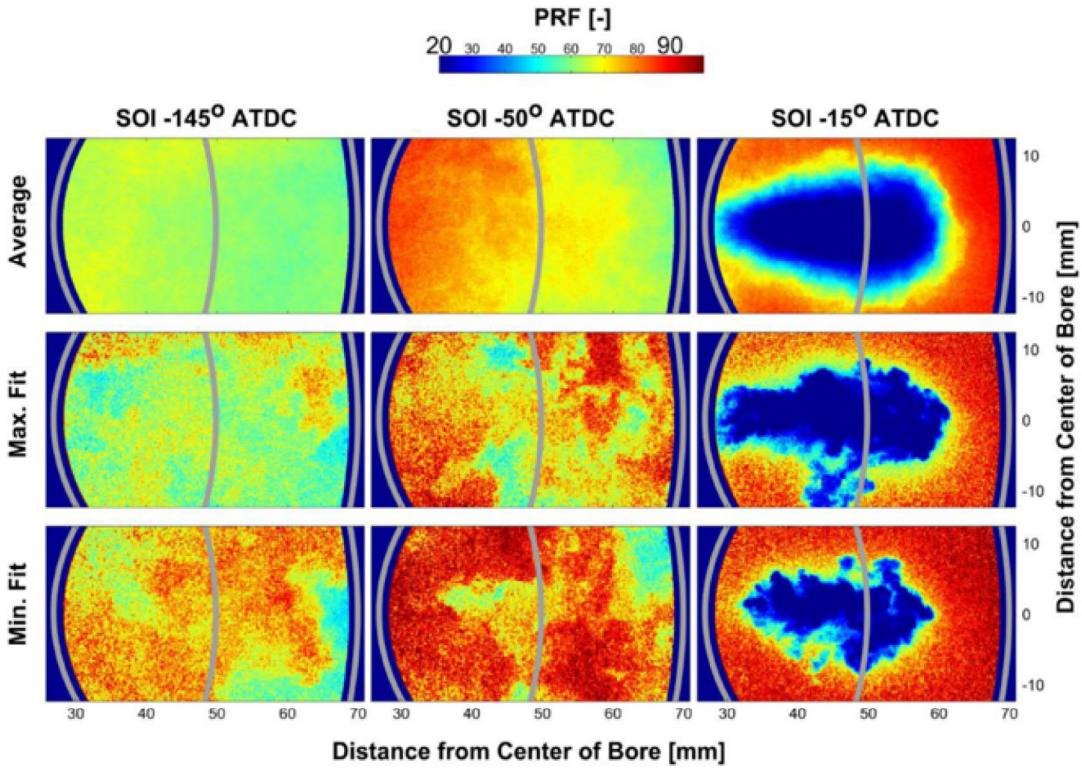


Figure 13: Iso-octane and N-Heptane Mixing Image, Average Mixing, Max.Fit Mixing and Min.Fit Mixing [33]

The numbers of diesel pulse affect the diesel distribution in the cylinder so that it influences fuel reactivity stratification. D. Splitter studied the injection effects in RCCI combustion [34]. The experiment compares single and double diesel injection

in four regions: diesel injection before 110° BTDC, 70°-110° BTDC, 40°-70° BTDC and after 40° BTDC, respectively. The results indicate that split diesel injections reduce CO and HC emissions by 40% and it leads to 1% thermal efficiency increasing. Single diesel injection usually results in higher peak HRR except for 50° BTDC experiment. Additionally, diesel-like combustion was found in late injection timings with high NOx emissions, which is mainly due to local λ and reactivity stratification. However, linear impingement occurs when the diesel injection is earlier than 70° BTDC. Y.P. Li summarise the characters of SOI and MSR showing in Fig.14. It can be concluded that at certain λ, diesel SOI and methanol fraction have influenced the combustion mode directly.

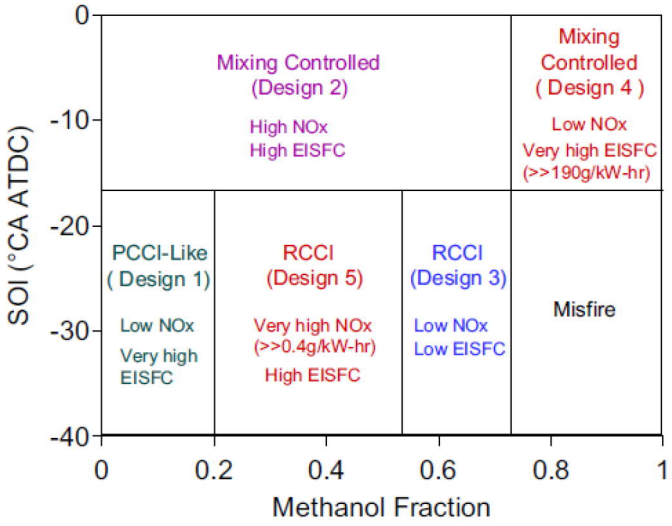


Figure 14: The Influence of Methanol Substitution Ratio and Diesel Start of Injection Timing on The Combustion Mode [35]

Compression ratio and Bowl geometry: From engine structure point of view, the compression ratio and bowl geometry have effects on RCCI combustion. NG/diesel RCCI experiments were conducted by Denbratt during which 14 and 17 compression ratio were used [31]. It is observed 14 compression ratio has longer ignition delay, combustion duration and lower peak HRR. While when the compression ratio is 17, knocking tends to occur at high load. Therefore, Denbratt concluded 14 compression ratio is more appropriate at high load operating conditions.

Bowl geometry has influences on air/fuel mixing and heat transfer, so it affects the thermal efficiency of RCCI combustion. D. Splitter improved the shape of the piston, and it can reduce the heat losses. It is also discovered by modifying the piston shape, RCCI brake thermal efficiency can be increased by 3% [31].

EGR rate: EGR has significant influences on the combustion temperature which additionally affects emissions. Principally, the feature of EGR is similar to low reactivity fuel, so in RCCI mode, EGR usage is expected to reduce. However, many

RCCI studies suggest high EGR is needed to stabilise RCCI combustion. Some results show the peak pressure rise rate is reduced by increasing the EGR rate [31]. Additionally, EGR rate significantly affects NOx emissions. It is discovered by Y. Li [35] that it is hard to maintain low NOx emissions by only increasing MSR. Y. Li also studied the relations between initial temperature and the amount of EGR needed. It is discovered with initial temperature increasing; higher EGR is required to keep high thermal efficiency and low NOx emissions. Fig.15 illustrates when the initial temperature reaches 410K, the EGR rate can be approximately 50%. The maximum amount of EGR rate is limited by the fuel consumption, and the low limit of EGR is engine knocking. Since fuel is more active when air intake temperature is high, which usually results in engine knock.

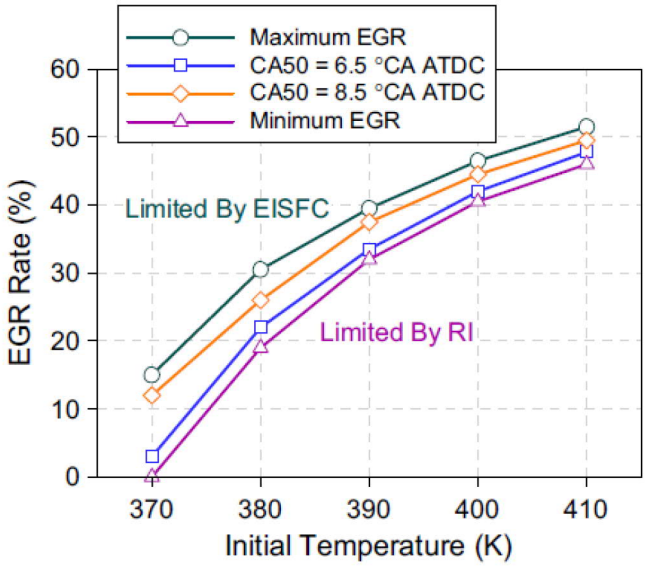


Figure 15: EGR Operation Range Under Different Initial Temperatures. Upper Limit: Equivalent Indicated Specific Consumption; Lower limit: Ringing Intensity [36]

2.4.2 Limiting Factors of RCCI

Knocking: Knocking is usually related to SI engine because of the end gas auto-ignition, but it can also occur in the RCCI combustion mode. When the temperature and pressure of the end gas reach the auto-ignition temperature, the premixed fuel burns rapidly before the flame propagation reaches such locations. Particularly, diesel is injected early in RCCI combustion, and the diesel particles presenting in the premixed region will induce the early combustion. The engine knocking results in swift in-cylinder pressure rise and unbalanced pressure wave which cause severe engine problems.

The knocking phenomenon is quantified by J.A. Eng [38] who summarised the ringing intensity (RI) of fuel is correlated with max. in-cylinder pressure, temperature and max. pressure rise rate (Eq.5).

$$RI = \frac{1}{2\gamma} \cdot \frac{(0.05(dP/dt)_{max})^2}{P_{max}} \cdot \sqrt{\gamma R T_{max}} \tag{5}$$

According to the numerical study done by D.Z. Zhou on methanol/biodiesel RCCI combustion, EGR is a practical approach to prevent engine knocking even at full load. Besides, the SOI of biodiesel is tested, and results show retarded SOI can also attenuate knocking. It is because there will be less premixed diesel in the cylinder if diesel SOI is delayed. Additionally, it is found more premixed methanol in the end gas tends to cause engine knocking [39]. Y. Li also studied the ringing intensity of methanol/diesel RCCI, and he concluded methanol/diesel combination has higher ringing intensity compared with gasoline/diesel at the same λ and air intake temperature. Due to the simple molecule structure, methanol prolongs the ignition delay. It means methanol and diesel have a longer time to mix homogeneously [40]. Evenly distributed methanol can effectively prevent early combustion of diesel. Although the use of methanol diminishes knocking to some degree, it still brings the upper limitations of operation load and maximum pressure rise rate.

Misfire: When methanol is not burning properly and most methanol slips, the phenomenon is referred to partial burning or even misfire. Several reasons are corresponding to incomplete burning or misfire in methanol/diesel RCCI combustion. Fuel mixing conditions are critical to RCCI combustion. If high reactivity fuel and low reactivity do not distribute evenly in the combustion chamber, the methanol may be exhausted before flame reaches the end gas. Methanol λ is another factor affecting methanol partial burning. Because of the flammability limitation, methanol does not burn in very lean conditions. However, many studies show that if methanol and diesel can mix homogeneously, methanol λ does not play an important role. Besides, air intake temperature is vital to methanol combustion, since it actives the fuel significantly. MSR is also considered as a reason for partial burning. When MSR is too high, the flame speed becomes slow due to sparse diesel particle distributions so that methanol partial burning occurs. Fig.14 indicates methanol misfire happens if MSR is greater than 75%.

2.4.3 Emission Characters of RCCI

The essential motivation of studying RCCI combustion is that theoretically, RCCI combustion can achieve low NOx and PM emissions due to low temperature combustion. While the high unburned hydrocarbon and CO emissions bring challenges to RCCI combustion. This section is going to analyse the formation of NOx, soot, unburned hydrocarbon and CO in standard diesel engines and how RCCI affects those emissions.

NOx: Nitrogen oxides (NOx) mainly refer to NO_2 and NO which is generated from both air and fuel in the combustion process. N constituent is negligible in diesel and methanol fuel and therefore, the NOx in the internal combustion engine is mostly derived from air. There are three paths to generate NOx: thermal NOx, prompt NOx and N_2O to NOx path. Thermal NOx is the most common path for NOx generation and the Zelodovich mechanism explains the formation of thermal NO:

$$\mathrm{O} + \mathrm{N_2} \rightleftharpoons \mathrm{NO} + \mathrm{N} \qquad \text{(k)}$$
$$\mathrm{O_2} + \mathrm{N} \rightleftharpoons \mathrm{NO} + \mathrm{O} \qquad \text{(l)}$$
$$\mathrm{N} + \mathrm{OH} \rightleftharpoons \mathrm{NO} + \mathrm{H} \qquad \text{(m)}$$

Fig.16 shows the temperature and ϕ conditions of NOx formation in the internal combustion engines. The high temperature is required for NOx generation. It is clearly illustrated in Fig.16 that NOx formation occurs when the local temperature is greater than 2200K. In terms of ϕ, the NOx is generated when the combustion is in stoichiometric or lean conditions. Diesel engine works under extra air conditions and the local jet combustion region is higher than 2200K. Therefore, the NOx emission is a severe issue of the diesel engine.

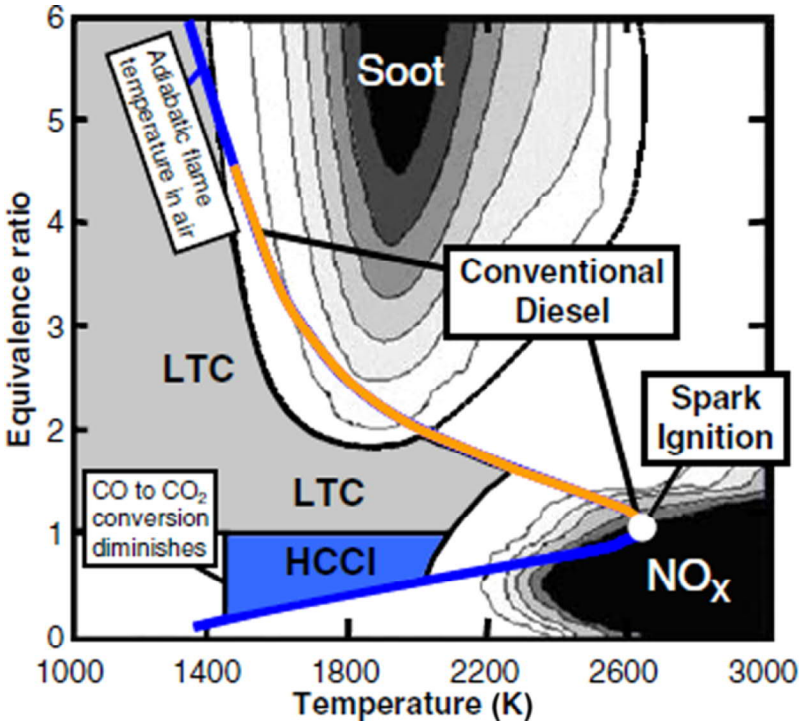


Figure 16: The Conditions of NOx and Soot Generation, ϕ-T Map [41]

Due to early diesel injection, the RCCI combustion avoids diesel rich high temperature. Although the combustion is taking place in relatively lean conditions, the low temperature effectively reduces the NOx formations.

PM: Particulate matter (PM) mainly contains soot which is generated in rich conditions. Fig.16 also shows the formation of soot that is generated between 1600K to 2200K temperature and fuel-rich conditions. In diesel combustion, polyaromatic hydrocarbons (PAH) is first produced in rich conditions, and PAH grows via conglomeration, subsequently, soot is formed. This process is shown in Fig.7. As analysed before, RCCI combustion circumvents the rich diesel jet. Hence, the soot emission can also be reduced.

Unburned HC: Unburned hydrocarbon (HC) is an issue concerning in premixed combustion, while there is much lower HC emission of diesel engine. The flame quenching is one of the main reason for HC emissions. In the RCCI combustion, methanol is premixed with air and in lean conditions. Thus, the lean condition and sparse methanol distribution can cause flame quenching. The flame cannot reach a part of end methanol. As a result, it increases not only CO emissions, but also increases the unburned methanol emissions.

CO: As shown in Fig.4, CO is an intermediate product and will eventually convert to CO_2. When the combustion temperature is too low, or the air is not efficient, the CO will fail to further convert CO_2. In this RCCI experiment, the methanol is in lean conditions (normally overall ϕ 0.44, methanol ϕ 0.25), so sufficient air present in the combustion chamber. However, the global temperature is low in RCCI combustion, which prevents the oxidation of CO. Hence, although RCCI combustion has positive effects on NOx and soot emissions, the CO and unburned hydrocarbon brings challenges to the technology.

3 Research Methodology

The majority part of the thesis is the LEO1 experiment and it is supported by methanol evaporation GT-SUITE simulation. The objective of GT-SUITE simulation is to understand the cooling effects of methanol vaporisation. Since both simulation and experiment are based on the all-metal engine, LEO1, the chapter will firstly introduce LEO1 configuration. Then, LEO1 based GT-SUITE model, LEO1 experimental methods and data post processing are instituted respectively in the following sections.

3.1 LEO1 Engine Setup

LEO1 research engine is based on AGCO SISU Power 84AWI 6-cylinder common rail off-road commercial heavy duty engine. The 6-cylinder engine is usually applied in the agricultural sector such as tractors. In total, the 6-cylinder engine has 8.42L displacement volume, while it is modified to a single cylinder research engine as LEO1. The engine is kept intact to maintain its balance. The piston pin is modified and a gap is left so that the piston will not compress air in other five cylinders. Table 2 lists LEO1 specifications.

Table 2: LEO1 Test Engine Specifications

Cylinder bore [mm]	111
Stroke [mm]	145
Displacement total [L]	8.4
Displacement 1-cyl [L]	1.4
Compression ratio	16.7

Fig. 17 illustrates LEO1 test engine setup. The LEO1 operation is not restricted by the commercial engine limitations since all the parameters including air intake temperature, exhaust pressure and injection timing can be freely manipulated. However, due to the free combination of variables, the in-cylinder combustion is not always stable. As a result, the power produced may be either too high to damage the engine or too low to maintain the set speed. Thus, an AC electric motor is connected to control the engine by either braking down the crankshaft or providing energy to keep the speed.

The parameters are controlled by a Field Programmable Gate Array from National Instruments and users get access to control the devices through customised LabView software. The engine operation information such as injection timing, injection duration and in-cylinder pressure is recorded by real time host-PC and then transferred to users' computer. Fuel system, air feeding, exhaust and Electrohydraulic valve actuator (EHVA) are the critical systems to control the engine parameters. The following section will specify those systems in detail for methanol/diesel RCCI experiment.

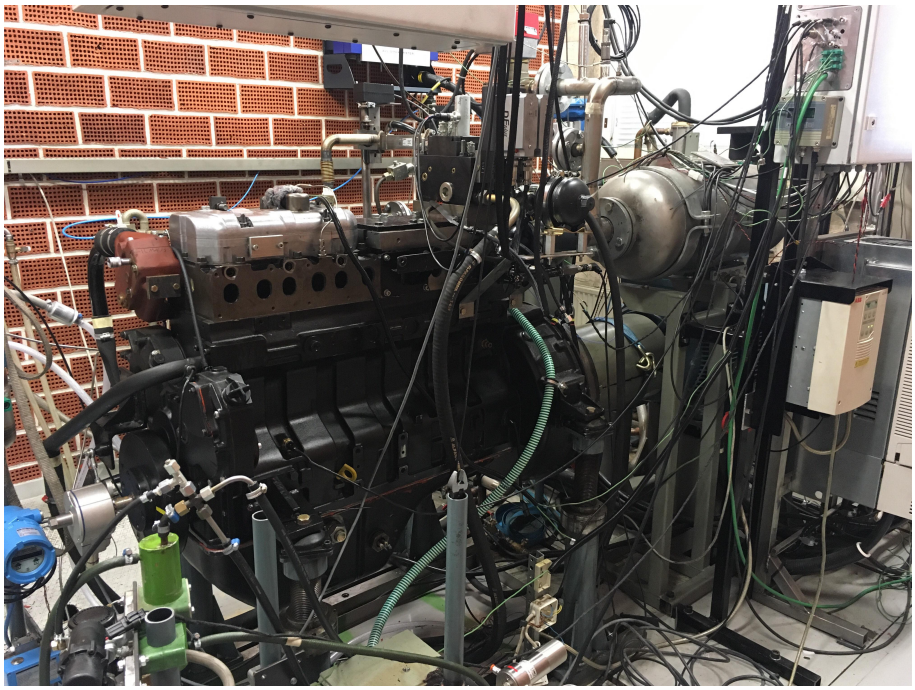


Figure 17: LEOI Test Engine Setup

3.1.1 Fuel System

The fuel system for RCCI experiment contains diesel injection system and methanol injection system. Diesel injection system includes fuel tanks, diesel fuel transfer pump, fuel filter, high pressure pump, common rail and diesel injector. Users control diesel injection parameters by LabView based engine control program. The rail pressure can be accurately changed between 800 to 2000 bars through a PID controller. The rail pressure is generated by an AC motorised high pressure pump with the frequency converter. DI driver module is used to control the diesel injector by specific given current.

The diesel injector is Bosch CRIN3-20 solenoid, high pressure DI for off-road heavy duty applications which follows Tier 4 Final standard. It is a 9-hole injector and each diameter is 0.138 mm. The DI driver module is able to reach the peak and hold current in 0.35 ms which is the minimum injection duration, but the diesel mass flow is unstable at this operation point. The operating pressure of the injector is 800 to 2000 bars and it is fixed at 1000 bar during the RCCI experiment. Fuel water cooling is equipped during the experiment since the fuel temperature is otherwise rising which affects the viscosity of the diesel, and subsequently influences the diesel mass flow. The diesel mass flow is calibrated from the measurements of a 1.5 kg Ohaus scale. The MSR is a crucial variable in the RCCI experiment so that the diesel mass flow has to be accurately monitored and controlled.

Methanol fuel system contains a fuel vessel, methanol transfer pump, fuel filter, methanol rail and methanol injector. The pressure sensor is installed at the methanol rail. The methanol rail has 3-5 bar pressure which is generated by methanol transfer pump and controlled by the regulator. The regulator keeps the pressure gap between methanol rail and manifold the same. The fuel is injected into the intake manifold mixing with air during the intake stroke.

Methanol injector is Bosch EV-14, conical spray injector. The injector has conically spray with spray angle between 15 to 85°. The maximum injection pressure is 8 bar and during the RCCI experiment, the methanol injection pressure is around 4 bar. The reference fuel flow is 1460 cc which is tested with n-heptane at 3 bar. More technical specifications are listed in Table 3 and methanol spray shape is shown in Fig.18.

Table 3: Methanol Injector Technical Specifications

System pressure [bar]	Max. 8
Operating temperature [°C]	-40 to 110
Permissible fuel temperature [°C]	Max. 70
Spray type	Conical Spray
Spray angle	15-85°
Fuel compatibility	E85/M100
Resistance [Ω]	12

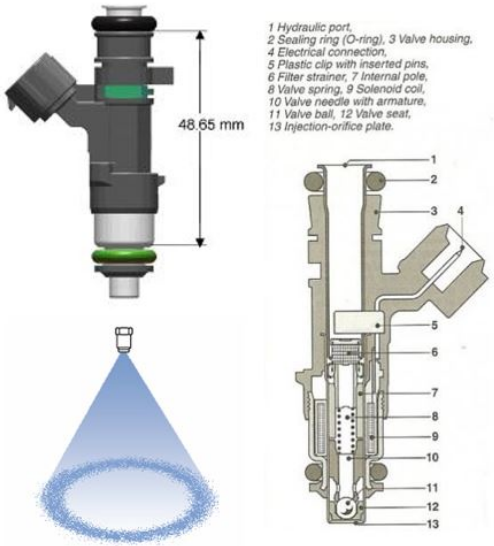


Figure 18: Methanol Injector and Methanol Spray

3.1.2 Air Feeding, Exhaust and EHVA system

The LEO1 research engine does not have a turbocharger apparatus, so an industrial air compressor is equipped to boost the charge air. The maximum air intake pressure is 8 bar. There is an electronic butterfly valve after the compressor to control the air mass flow. The position of the butterfly valve is set by a PID controller via LabView software. To reach the test conditions, the users can set the required air mass flow or needed boost pressure. In the RCCI experiment, air mass flow is controlled and the charge air pressure is between 1.2 to 1.4 bar. An external heating core is placed after the butterfly valve to adjust air intake temperature and the highest air intake temperature is 70°C. The exhaust side contains a pulse absorber and a back pressure valve. By changing the back pressure, the LEO1 research engine can simulate turbocharger.

An Electrohydraulic valve actuator system (EHVA) is implemented to LEO1 which can adjust the valve lifting profile by high pressure hydraulic fluid. It allows users to define the intake and exhaust valve lifting profile without changing any hardware or physical components. To summarise, the test configuration of LEO1 is shown in Fig.19.

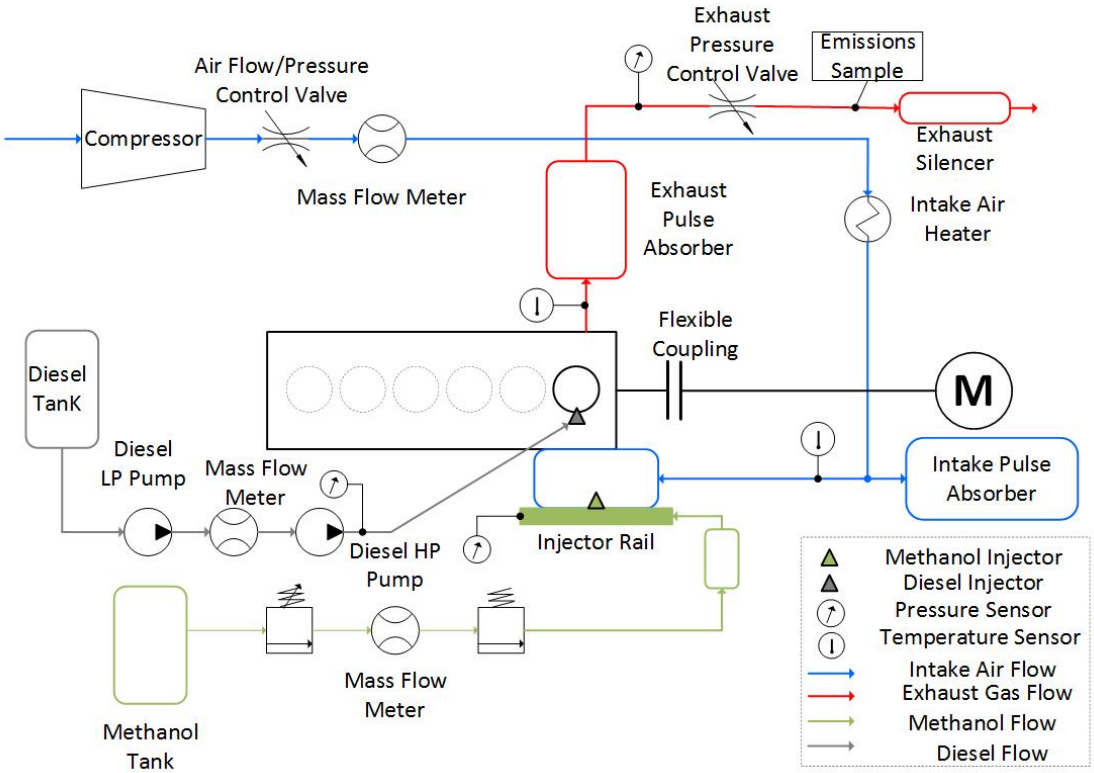


Figure 19: LEO1 Test Configuration

3.2 GT-SUITE Simulation of Methanol Evaporation

Due to the high latent heat of vaporisation (1150 MJ/kg), methanol evaporation brings significant cooling effects to the cylinder. Although the cooling impact increases the ringing intensity of the charge, it negatively affects fuel ignition and increases the HC emissions. Therefore, it is necessary to investigate the methanol evaporation quantitatively. GT-SUITE is used to model LEO1 engine, particularly, methanol injection process. The in-cylinder temperature at top dead centre (TDC) and the temperature at intake valve close (IVC) are calculated.

Simulation has been done in GT-SUITE v2017 and results are analysed in GT-Post v2017. The objective is to understand the methanol evaporation, so diesel injection and combustion are not modelled in this case. Fig.20 illustrates the model of LEO1 one-cylinder research engine with methanol injector. On the one hand, inlet side has 1.3 bar intake pressure and intake temperature varies from 40°C to 70°C; intake flow is split into two streams because practically LEO1 has two intake ports. Methanol injector controls methanol injection timing and injection rate. On the other hand, exhaust side has 1.2 bar pressure and 30°C outlet temperature. The other parameters are based on LEO1 research engine and Table 4 illustrates vital parameters of the GT-SUITE model [13].

Table 4: Parameters of GT-SUITE Model

Charge air pressure [bar]	1.3
Exhaust pressure [bar]	1.2
Exhaust temperature [°C]	30
Methanol temperature [°C]	20
Engine speed [RPM]	1500
Compression ratio	16.7

In this GT-SUITE model, the phase change is defined in the two components: methanol injector and engine cylinder. Methanol injector defines a vaporised fluid fraction which means the amount of methanol evaporates immediately after injection. According to the database of GT-SUITE, the typical value for gasoline is 0.3, so the vaporised fluid fraction of methanol can be calculated based on the latent heat of these two fuels in Eq.6. The latent heat of gasoline is 350 MJ/kg, and the data of methanol is 1150 MJ/kg. Thus, the coefficient of methanol vaporisation is 0.0913.

$$0.3 \times L_{gasoline} = C_{vff} \times L_{methanol} \tag{6}$$

Engine cylinder evaporation objective defines the methanol model in the engine cylinder. It can be specified as a profile where methanol evaporation fraction is a function of crank angle or use the model "50% Evaporation Duration (CAD)". This "half-life model" was studied by Paul N. Blumberg and presented in GT-SUITE users conference in 2009 [37]. The results of E85 illustrates that 25 CAD ‘half-life

model' is accurate enough compared with experimental results. The only concern is that the data of E85 might not be accurate for methanol, so this value is varied during the simulation. However, the results show that temperature is not sensitive to this parameter, hence 25 CAD is used in the thesis's GT-SUITE model.

Engine heat transfer model WoschniGT refers to B. Heywood's research of the cylinder heat transfer, conduction, convection and radiation are considered in WoschniGT model, but it does not consider swirl in the cylinder [21].

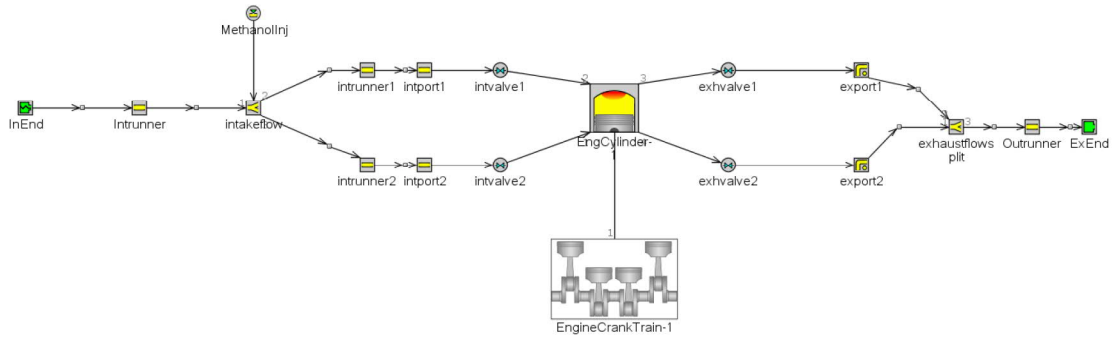


Figure 20: GT-SUITE LEO1 Model of Methanol Evaporation

3.3 LEO1 Experimental Methods

3.3.1 Test Methods

There are limited numbers of methanol/diesel RCCI experimental studies available, though it has been widely numerically studied. Hence, the methanol/diesel RCCI thesis aims at presenting broad and reliable test results of most key parameters. A systematic test method and well-organised test matrix must be defined. In this experiment, the key variables are Air mass flow (AMF), Air intake temperature (AIT), Methanol injection timing (MIT), Diesel injection timing (DIT) and Methanol substitution rate (MSR). For each parameter, the test is divided into the following four steps:

Experimentation Preparation: Experiment preparation includes engine warm up and important systems checking. It contains EHVA system checking, engine cooling water preparation, air compressor starting, fuel level inspection, emission calibrating and so forth. After a series of tasks, the engine can start to rotate and experiment ready to carry on.

Test Matrix Reviewing: Text matrix must be modified based on the previous experiment results. Since experiment results do not always follow the expectations,

test points must be adjusted. For example, to study the influence of air intake temperature, all other parameters should be the same in different temperature points which are set as 20°C, 30°C and 40°C initially. However, the start of ignition is too early in 40°C air intake case and the SOI has to be adjusted. As such, the temperature step should be changed smaller to 20°C and 25°C.

Combustion Stabilisation and Data Recording: Only the test point with stable combustion are regarded as valid points. Specifically, stabilised combustion refers to pressure rising occurs around TDC without sharp pressure increasing and pressure fluctuation, as well as constant NOx level. After the combustion is stabilised, cylinder pressure of at least forty cycles is recorded. The engine operating conditions such as air mass flow, air intake temperature, methanol and diesel injection information are saved as well.

Data Analysing: The recorded data is analysed by Matlab 2017a and the calculation methods refer to *"International Combustion Engine Fundamentals"* by Heywood. The calculation details are introduced in Section 3.4.

3.3.2 Parameters Setup and Test Matrix

As discussed in section 2.3, diesel injection strategy is fundamentally crucial to RCCI combustion. The experiment is hence divided into two groups: single diesel injection experiments and split diesel injection experiments. In the split diesel injection experiments, early diesel injection event is named as premixed diesel and the second diesel pulse is designated as pilot diesel in the experiment.

Study of Split Diesel Injection
Case 1: Study of Methanol Injection Timing: The influence of methanol injection timing is studied by setting up methanol injection timing at 340°, 360° and 390° BTDC. Diesel is delivered at the same time in all three test points, that the premixed diesel is injected at 50° BTDC and the pilot diesel is injected at 11° BTDC. It should be mentioned the premixed diesel is injected as early as possible to create homogeneous mixtures, but not too early to wet the piston wall. 3.44 kg/h methanol mass and 1.37 kg/h diesel fuel are injected, which totally contain 2.85 kJ/cycle energy and MSR is 54%. The test is conducted at ambient conditions (AIT 18°C) and air mass flow is 100 kg/h providing ϕ 0.42. Test specifications are listed in Table 5.

Table 5: Test Specifications of Case 1: Methanol Injection Timing

	MIT [CAD]	DIT [CAD]	MSR	Fuel Energy [kJ/cycle]	ϕ
Test1-1	340 BTDC	50/11 BTDC	54%	2.85	0.42
Test1-2	360 BTDC	50/11 BTDC	54%	2.85	0.42
Test1-3	390 BTDC	50/11 BTDC	54%	2.85	0.42

Case 2: Study of Air Mass Flow (ϕ): At the ambient air intake temperature conditions, five air mass flow 80, 90 100, 110 and 120 kg/h are chosen to investigate the influence of ϕ. Except for air mass flow, all other parameters are kept the same in the test. Methanol is injected at 340° BTDC, premixed diesel is delivered at 50 ° BTDC and pilot diesel is injected at 13° BTDC, respectively. 3.59 kg/h methanol and 1.38 kg/h diesel are used in each test point which contains 2.93 kJ/cycle fuel energy. The methanol substitution rate is 55% in all the test points, which means methanol ϕ is changing as well. The important parameters are shown in Table 6.

Table 6: Test Specifications of Case 2: Air Mass Flow

	AMF [kg/h]	ϕ	Methanol ϕ	MSR	Fuel Energy [kJ/cycle]
Test2-1	80	0.55	0.29	55%	2.93
Test2-2	90	0.49	0.26	55%	2.93
Test2-3	100	0.42	0.23	55%	2.93
Test2-4	110	0.39	0.21	55%	2.93
Test2-5	120	0.36	0.19	55%	2.93

Case 3: Study of Air Mass flow at 70°C: The combustion behaviour is additionally explored at 70°C air intake temperature conditions. The air mass flow of 80, 90 and 100 kg/h are studied. All the parameters are the same as Case2 except the diesel injection timing. The premixed diesel is delivered at 50° BTDC, but the pilot diesel is injected at 9° BTDC in all three test points. Table 7 lists the key parameters of this case.

Table 7: Test Specifications of Case 3: Air Mass Flow at 70°C

	AMF [kg/h]	ϕ	Methanol ϕ	MSR	Fuel Energy [kJ/cycle]
Test3-1	80	0.54	0.29	54%	2.92
Test3-2	90	0.48	0.26	54%	2.92
Test3-3	100	0.43	0.23	54%	2.92

Case 4: Study of MSR at different Engine Load: Methanol substitution rate is studied at two load conditions: 7.5 bar IMEP (2.89 kJ/cycle fuel energy) and 12 bar IMEP (4.44 kJ/cycle fuel energy). The experiment is conducted at 40°C air intake temperature because the previous results show 40°C is promising for the RCCI combustion concerning ignition and ringing intensity. Air mass flow at middle load condition is 80 kg/h, and it is adjusted to 120 kg/h at high load case to keep ϕ the same. Methanol is delivered at 340° BTDC in both load points. The first diesel injection in both loads is 50° BTDC, while the second diesel injection for middle load test and high load test are 11° BTDC and 9° BTDC, respectively. Test specifications of Case 4 are shown in Table 8 and Table 9.

Table 8: Test Specifications of Case 4: Methanol Substitution Rate at Middle Load

	Fuel Energy [kJ/cycle]	MSR	ϕ	AMF [kg/h]
Test4-1	2.84	27%	0.53	80
Test4-2	2.84	36%	0.53	80
Test4-3	2.84	40%	0.53	80
Test4-4	2.84	55%	0.53	80

Table 9: Test Specifications of Case 4: Methanol Substitution Rate at High Load

	Fuel Energy [kJ/cycle]	MSR	ϕ	AMF [kg/h]
Test4-5	4.38	38%	0.53	120
Test4-6	4.38	47%	0.53	120
Test4-7	4.38	63%	0.53	120

Study of Single Diesel Injection

Case 5: Study of Methanol Injection timing: Similar as split diesel injection, the methanol injection timing is also studied in the single diesel injection experiment and MIT 320°, 340°, 360° and 390° BTDC are applied in the test. Diesel is delivered at 28° BTDC. The fuel contains 2.83 kJ/cycle energy in total, and MSR is 54% in all experiments. Air mass flow is 100 kg/h at ambient intake temperature which gives ϕ as 0.44. Table 10 indicates variables in this test.

Table 10: Test Specifications of Case 5: Methanol Injection Timing

	MIT [CAD]	DIT [CAD]	MSR	Fuel Energy [kJ/cycle]	ϕ
Test5-1	320 BTDC	28 BTDC	54%	2.83	0.44
Test5-2	340 BTDC	28 BTDC	54%	2.83	0.44
Test5-3	360 BTDC	28 BTDC	54%	2.83	0.44
Test5-4	390 BTDC	28 BTDC	54%	2.83	0.44

Case 6: Study of Air Intake Temperature: AIT at 20°C and 25°C are compared in this case. Total fuel energy is still approximate 2.89 kJ/cycle, but MSR is set up at 47%. It is because lower MSR at low air intake temperature can reduce methanol slip effectively. Diesel is injected at 36° BTDC and methanol is delivered at 320° BTDC. Table 11 lists the test specifications of this case.

Table 11: Test Specifications of Case 6: Air Intake Temperature

	AIT [°C]	DIT [CAD]	MSR	Fuel Energy [kJ/cycle]	ϕ
Test6-1	21	36 BTDC	47%	2.87	0.43
Test6-2	25	36 BTDC	47%	2.87	0.43

Case 7: Study of Diesel Injection Timing for different MSR: After the previous experiments, it has been discovered the diesel SOI varies significantly for different fuel reactivities. Therefore, this case focuses on the diesel SOI at different methanol substitution rate. The air intake temperature is ambient (18°) for all test points and air mass flow is constant at 100 kg/h. Methanol is injected at 320° BTDC and total fuel energy is 2.89 kJ/cycle. 37%, 49%, 58%, 62% and 70% MSR are studied in the experiment. Diesel injection timing for each MSR is listed in Table 12.

Table 12: Test Specifications of Case 7: Diesel SOI for Differernt MSR

	MSR	DIT [CAD]			MIT [CAD]	Fuel Energy [kJ/cycle]	ϕ
Test7-1	37%	52	54	56	320 BTDC	2.89	0.44
Test7-2	49%	34	34.5	35.5	320 BTDC	2.83	0.43
Test7-3	58%	29	29.5	30.5	320 BTDC	2.68	0.42
Test7-4	62%	24.5	25	26	320 BTDC	2.73	0.42
Test7-5	70%	15	20	21	320 BTDC	2.67	0.40

3.4 Data Processing

3.4.1 Fuel Related Parameters and Calculations

Methanol mass flow rate ($\dot{m}_{methanol}$), diesel mass flow rate ($\dot{m}_{diesel}$) and air mass flow ($\dot{m}_{air}$) are measured during the experiment. Therefore, the energy flow rate and fuel substitution can be calculated.

Calculate energy flow rate $\dot{E}$ from Eq.7, where $\dot{m}_f$ stands for fuel mass flow.

$$\dot{E} = \dot{m}_f \times LHV \tag{7}$$

With the known energy flow rate, the energy substitution ratio of each fuel can be calculated. Eq.8 expresses the diesel substitution ratio (DSR).

$$DSR = \frac{\dot{E}_{diesel}}{\dot{E}_{methanol} + \dot{E}_{diesel}} \tag{8}$$

While in RCCI combustion, the fuel reactivity level is adjusted by methanol continent and usually methanol accounts for more than 50% energy, so instead of DSR, MSR is more used in the thesis. The calculation formula is shown in Eq.3.

AFR and λ is defined as the same as diesel or gasoline combustion, but due to two fuels used in the RCCI combustion, the expression is different. Total AFR, methanol AFR and diesel AFR are calculated from measured fuel mass flow and air mass flow. Subsequently, methanol λ and diesel λ at that quantity can be derived from real AFR and stoichiometric AFR, shown in Eq.11 and Eq.12 respectively. Equivalent ratio, the revise of λ, is used as an indicator of the air-fuel mixture in the RCCI thesis (Eq.13).

$$AFR_{tot} = \frac{\dot{m}_{air}}{\dot{m}_{methanol} + \dot{m}_{diesel}} \tag{9}$$

$$\lambda = \frac{AFR_{tot}}{AFR_{stoichiometric}} \tag{10}$$

$$\lambda_m = \frac{AFR_{methanol}}{AFR_{m,st}} \tag{11}$$

$$\lambda_d = \frac{AFR_{diesel}}{AFR_{d,st}} \tag{12}$$

$$\phi = \frac{1}{\lambda} \tag{13}$$

3.4.2 Cylinder Temperature, Pressure and Heat Release Calculation

Heywood assumes the compression stroke in the CI engine is an isentropic process [21] and therefore, the temperature at TDC can be calculated by Eq.14.

$$\frac{T_{TDC}}{T_1} = (\frac{P_{TDC}}{P1})^{\frac{\gamma-1}{\gamma}} \tag{14}$$

Where T_1 stands to intake temperature, P_1 represents intake pressure and γ is the ratio of air specific heats. In this calculation, γ uses 1.35.

Heat release analysis reflects the combustion rate and the combustion phase which is widely used to quantify the engine combustion process. It is calculated from recorded in-cylinder pressure via thermodynamics principles. To acquire the heat release rate, the calculation assumes the in-cylinder charge as the ideal gas. Applying the first law of thermodynamics for an open system, the energy balance can be written as:

$$\frac{dQ}{d\theta} - P\frac{dV}{d\theta} + \sum_i \dot{m}_i h_i = \frac{dU}{d\theta} \tag{15}$$

Where Eq.15 represents the change of the internal energy which is equal to the heat absorbed by the system and the energy content entering the system diminishing the

work done by the system. However, the system is a quasi-static, and it is not possible to apply Eq.15 to the engine cylinder. Thus, apparent heat release calculation is used to estimate in-cylinder heat release (Eq.16).

$$\frac{dQ}{d\theta} - P\frac{dV}{d\theta} + \dot{m}_f h_f = \frac{dU}{d\theta} \tag{16}$$

Where $dQ/d\theta$ refers to gross heat release. If heat transfer through the in-cylinder wall is neglected, the apparent net heat release of the charge in the cylinder is:

$$\frac{dQ_n}{d\theta} = \frac{dQ_{gross}}{d\theta} - \frac{dQ_{ht}}{d\theta} = P\frac{dV}{d\theta} + \frac{dU}{d\theta} \tag{17}$$

Applying the ideal gas law (PV=nRT) the Eq.17, the heat release rate versus crank angle can be finally expressed as:

$$\frac{dQ_n}{d\theta} = \frac{\gamma}{\gamma - 1}P\frac{dV}{d\theta} + \frac{1}{\gamma - 1}V\frac{dP}{d\theta} \tag{18}$$

It should be mentioned that the in-cylinder gas is not ideal gas since the pressure in the combustion is high, and therefore, the ideal gas calculation brings the error to the heat release analysis. However, it is hard to control the complicated gas equations in real conditions and if the real gas calculation is applied, the heat release calculation from different laboratories, companies are not comparable. Besides, the ideal gas calculation does not affect the shape of the heat release curve. Thus, the ideal gas based calculation is widely used in the engine-related analysis.

By summing up the heat release in each stage from the start to the end of the process, cumulative heat release (QHR) can be obtained:

$$QHR = \sum_{i=m}^{n} (\frac{dQ_n}{d\theta})_i \tag{19}$$

The pressure rise rate (PRR) which is critical to identify the engine knocking can be calculated by Eq.20.

$$PRR = \frac{dP}{d\theta} \tag{20}$$

Thermal efficiency is also estimated in the experiment. Since only indicate power can be acquired, the efficiency refers to indicated thermal efficiency (ITE) which is calculated from indicate power and fuel energy input:

$$ITE = \frac{P_{indicate}}{E_{fuel}} \tag{21}$$

4 Results and Discussion

4.1 GT-SUITE Results of Methanol Evaporation

Fig.21 left shows the in-cylinder temperature at TDC after compression stroke. It can be observed that the maximum temperature increases significantly with methanol substitution decreases. When methanol replaces all diesel fuel, the peak temperature is less than 400°C regardless of air intake conditions. By contrast, when methanol substitution reduces to 50%, highest temperature in all four cases exceeds 500°C. Furthermore, the TDC temperature is rising with the increase of air intake temperature.

The tendency of the temperature curve at IVC (Fig.21 right) is the same as that at TDC. The IVC temperatures are negative in four cases when methanol substitution rate is 100%. To maintain the IVC temperature higher than 0°C, the methanol substitution rate must be lower than 70%. With the methanol substitution rate decreasing, the IVC temperature keeps rising and overreaches 60°C in all cases.

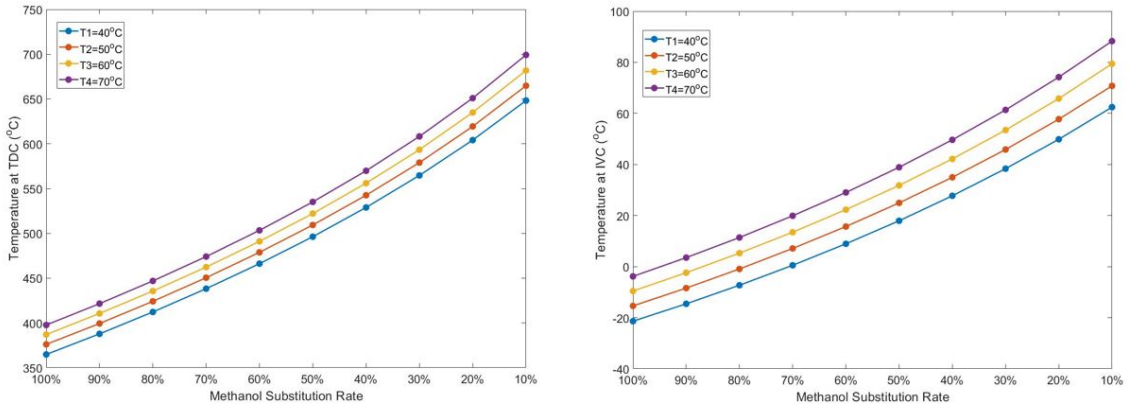


Figure 21: Methanol Evaporation GT-SUITE Simulation Results

The simulation results suggest that higher air intake temperature diminishes the effects of methanol evaporation, and subsequently increases the in-cylinder temperature. To validate and further investigate the influences of air intake temperature, RCCI experiments are conducted at a range of air intake temperatures ranging from 18°C to 70°C.

It should be mentioned that only one methanol injector was used in the real experiment. It is because of the shape of the intake manifold that one gas path is straight and direct to the intake valve while another path is bent. It brings wall wetting problems for methanol injection and therefore, the only direct path was used in the experiment.

4.2 Split Diesel Injection Experiment Results

4.2.1 Case 1: Effects of Methanol Injection Timing

Split diesel injection methanol/diesel RCCI combustion shares similar heat release characters. The pressure and HRR curve of Test1-1, Case 1 is illustrated in Fig.22. Two-stage heat release clearly occurs: the rapid heat release starting from TDC followed by a slower and longer duration heat release. To understand the combustion mechanisms, the combustion conditions must be mentioned. The Test1-1 has 54% MSR, so the energy from diesel is 46%, among which 24% diesel is delivered in pilot injection and 22% is premixed with methanol. CA24 and CA46 represent 24% heat release and 46% heat release which are marked in Fig.22. Thus, this two-stage heat release contains three combustion phases: (I) pilot diesel combustion, from CA5 to CA24. In this stage, heat release results from the pilot diesel combustion (II) premixed diesel particles combustion and ignite methanol, CA24 to CA46. During this stage, the premixed diesel starts to burn and ignite the surrounding methanol. Yet the heat release rate is lower than the pilot diesel because the condition for premixed diesel is lean. (III) Premixed methanol combustion, CA46 to CA90. The methanol in the remaining end gas is burned and releases heat in the last stage. The methanol burning rate is slower than diesel combustion because the methanol has lower reactivity level and the condition is lean. Since the pilot diesel injection is always delivered close to TDC, similar combustion behaviours are observed in most of split diesel RCCI case.

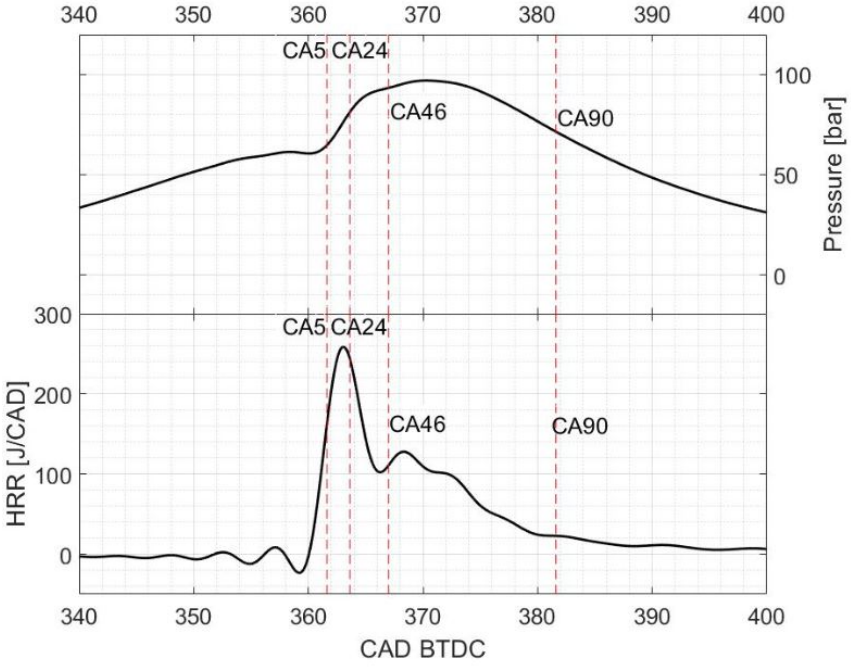


Figure 22: Combustion Characters of Split Diesel Injection. Premixed Diesel Injection Timing: 50° BTDC; Pilot Diesel Injection Timing: 11° BTDC

The cylinder pressure and HRR curve of Test1-1, Test1-2 and Test1-3 are shown in Fig.23. It can be observed that the methanol injection timing does not affect the combustion phase because the heat release characters are the same in all three test points. However, CA5 is more advanced in early methanol injection case and the ignition delay in 390° BTDC is the shortest. It is because early methanol injection creates a more homogeneous mixture which benefits the flame propagation. Besides, the intake valve opens at 370° BTDC, so if methanol is injected before intake valve open (Test1-3, 390° BTDC), the methanol does not absorb heat in the combustion to evaporate. The negative influence of methanol evaporation is diminished. ITE is also calculated, and the results show the ITE reduces with methanol injection timing advanced. However, the range of ITE is less than 0.5%, so the effects are negligible.

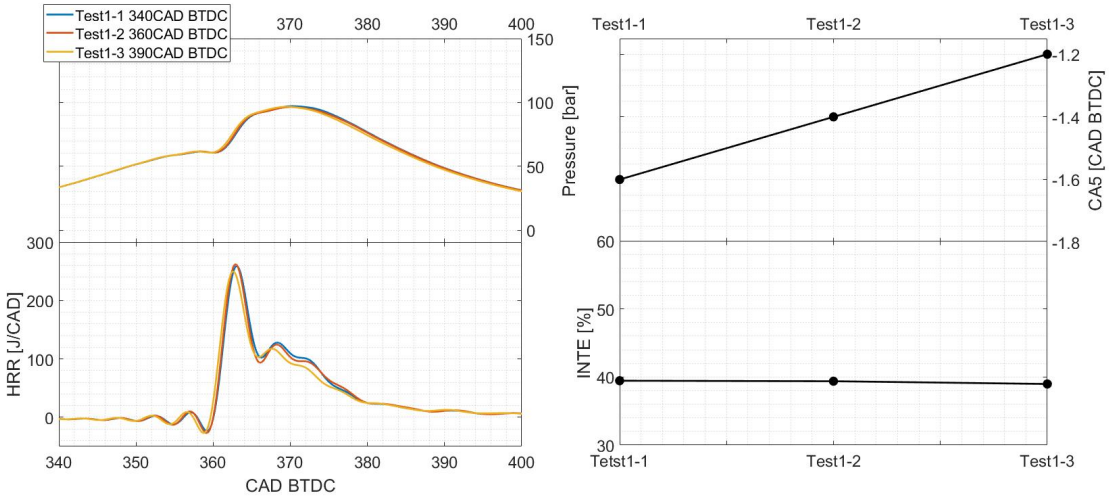


Figure 23: Effects of Methanol Injection Timing

4.2.2 Case 2: Effects of Air Mass Flow (ϕ)

The air mass flow or ϕ influence combustion phase directly, since the HRR curve shows different behaviours in five test points (Fig.24). There is only one peak showing in Test2-1, while all other tests points have two-stage heat release. The combustion in Test2-3, Test2-4 and Test2-5 are similar to the combustion in case 1, that the first stage heat release results from diesel pilot and the slow heat release is from the premixed end gas. By contrast, only one stage heat release can be observed in Test2-1 (80 kg/h air mass flow). It is because the fuel is more active under rich conditions so that the combustion starts simultaneously at different locations in the cylinder leading to synchronous heat release. In test2-2 (90 kg/h air mass flow), the combustion of diesel pilot and end gas have an noticeable gap, but the combustion

rate in the second stage is almost the same as the first stage. It suggests the heat release in the second stage is only from premixed diesel the estimation of fuel conversion rate is only 77% which additionally indicate most methanol fuel is not burning in this air mass flow condition. In other words, the premixed flame propagation has no time to fully develop in Test2-2 states.

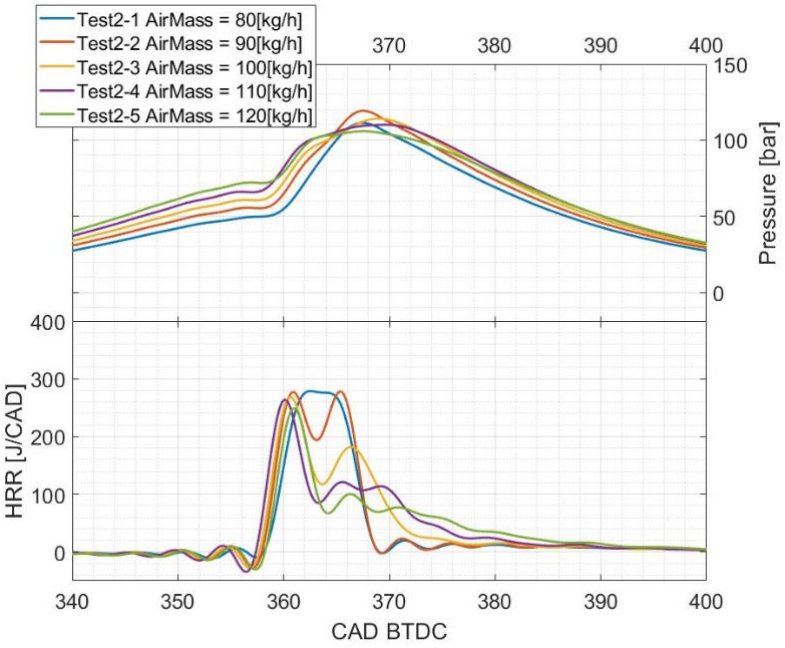


Figure 24: Effects of Air Mass Flow (ϕ)

Knocking occurs in Test2-3, Test2-4 and Test2-5, which results in higher ITE than Test2-1 and Test2-2. The unfiltered pressure curve of test2-3 is illustrated in Fig.25.

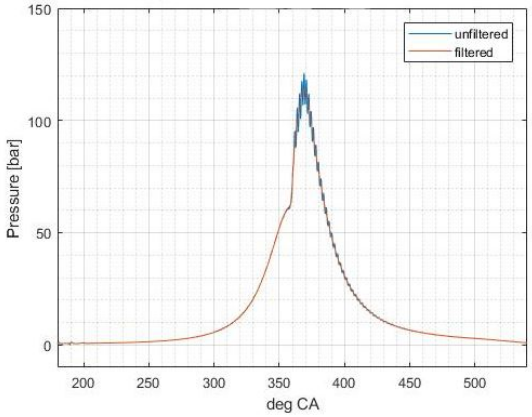


Figure 25: Unfiltered Pressure of Test2-3

4.2.3 Case 3: Effects of Air Mass Flow at 70°C

Compared with ambient air intake conditions, the combustion behaviour of different air mass flow is uniform when air intake temperature is 70°C. As shown in Fig.26, the pressure rises suddenly in all three test points and the maximum PRR is over 23 bar/CAD in 80 kg/h air mass flow experiment. The heat releases aggressively and the combustion duration is extremely short. It can be seen the high air intake temperature has a significant influence on the combustion. In this air intake temperature, the premixed charge is ignited immediately after the pilot diesel injection. As a result, the diesel diffusion flame and premixed flame cannot be distinguished.

Strong knocking is observed in 80 kg/h air mass flow test, which is the reason for such a short combustion duration. The leaner conditions can prolong the combustion duration and stabilise the combustion. The ignition timing is all three test points are similar, while the ITE is improved with air mass flow increasing.

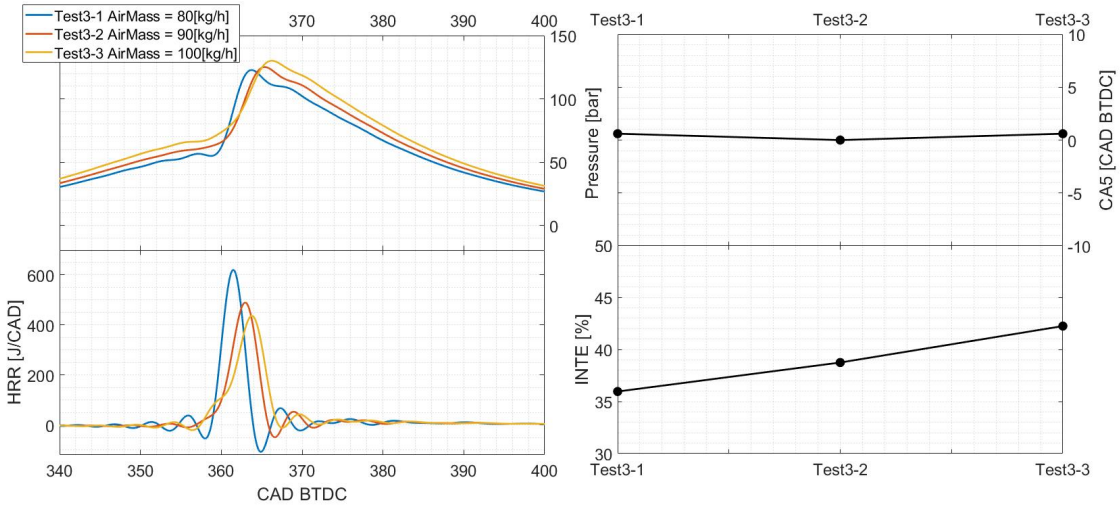


Figure 26: Effects of Air Mass Flow at 70°C

Comparing *Case1: Effects of Air mass flow at ambient temperature* and *Case2: Effects of Air Mass flow at 70° C*, the following points are summarised. By increasing the air intake temperature, the fuel reactivity level has been significantly improved. Practically, it behaves as rapid combustion of the end gas which almost burns with pilot diesel at the same time. As a result, the combustion duration is much shorter in high air intake temperature. To reduce the aggressive pressure rise and heat release, the condition must be leaner, or the air intake temperature is lower.

4.2.4 Case 4: Effects of MSR at different Engine Load

The effects of methanol substitution rate are investigated in both middle load and high load conditions. The middle load refers to around 40% of the full load of LEO1 which corresponds to 2.89 kJ/cycle fuel energy and the high load indicates the 70% of the full load of LEO1 which contains 4.44 kJ/cycle fuel energy. As shown in Fig.27, the combustion behaviour is very different in high load experiments where clear premixed flame propagation can be seen. In Test4-5, Test4-6 and Test4-7, the combustion of diesel pilot results in the first stage heat release. It also ignites the premixed charge which contains both methanol and diesel leading to the second stage heat release. The heat release from the premixed charge is rapid in high load tests because the methanol is mixed homogeneously so that the combustion starts simultaneously at different locations. Besides, the ϕ in this group of the experiment is 0.55, so the condition is relatively rich. Thus, the premixed charge shows rapid combustion behaviour instead of slow and long duration combustion demonstrated in Fig.22 Additionally, the combustion is retarded with MSR increases and higher pressure is reached in high MSR test points.

While in middle load conditions, the premixed flame propagation can be distinguished clearer in high MSR tests, especially in Test4-4. It is because when MSR is low, the methanol continent entering diesel diffusion flame regions and the combustion is similar to diesel combustion. When the MSR increases, the second stage heat release is governed by the methanol component. Same as high load experiment, the combustion is retarded and ignition delay is increased with increasing of MSR.

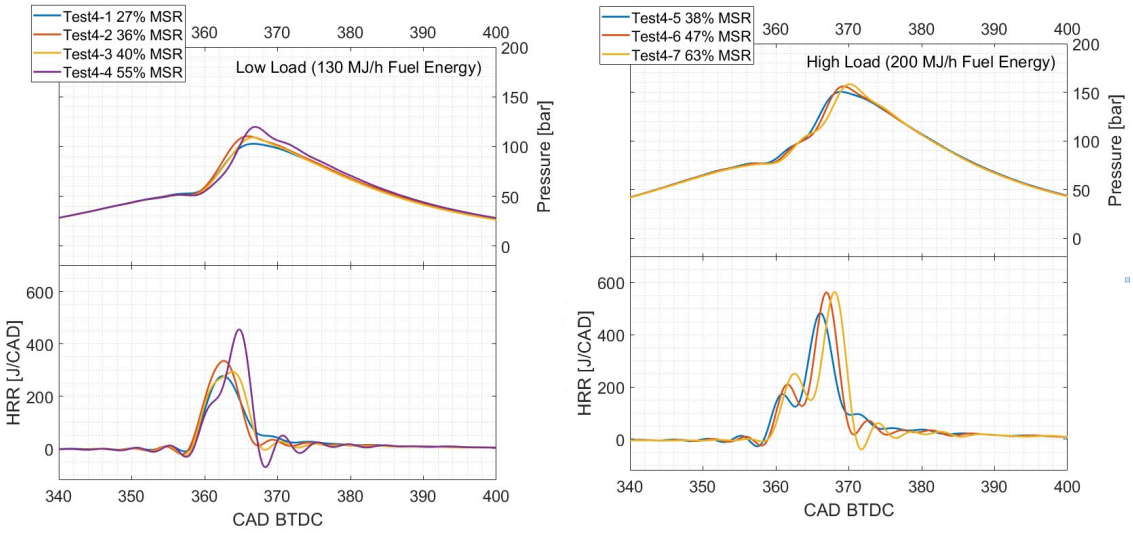


Figure 27: Effects of MSR at Different Engine Load

4.3 Single Diesel Injection Event Experiment Results

4.3.1 Case 5: Effects of Methanol Injection Timing

Fig.28 shows the pressure and heat release curve of Test5-1 which represents typical heat release characters of single diesel injection experiments. There are also two stages of heat release: low temperature heat release from 350° BTDC to around 356° BTDC and high temperature heat release which is right after LTHR. Diesel is delivered at 28° BTDC and it mixes with methanol evenly. Compared with split diesel injection where the pilot diesel brings significant diffusion flame propagation, the single diesel injection experiments show the in-cylinder charge burns homogeneously leading to one stage main heat release. Specifically, the diesel fuel distributed in cylinder charge results in LTHR and subsequently triggers HTHR of premixed charge. This combustion behaviour is observed in all single diesel injection test points.

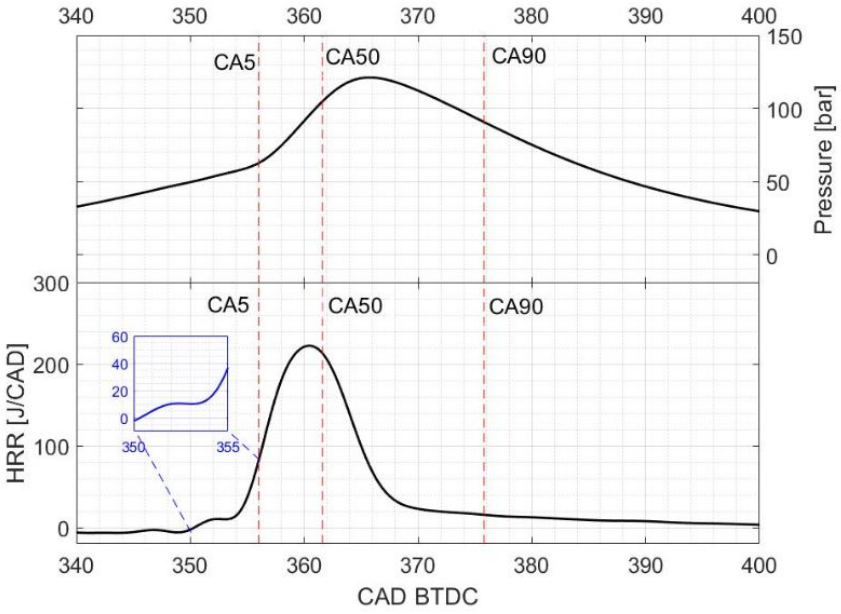


Figure 28: Combustion Characters of Single Diesel Injection. Diesel Injection Timing: 28° BTDC.

The effects of methanol injection timing in single diesel experiments are similar to split diesel experiments, that methanol injection timing does not have considerable influence on the combustion behaviours and indicate thermal efficiency (Fig.29). However, it is observed the peak pressure and peak HRR of early methanol injections (Test5-3 and Test5-4) are lower than the late methanol injection case. More specific, when injecting methanol at 390° BTDC, the combustion starts early (CA5 at 4.6° BTDC). While if methanol is delivered at 360° BTDC, the combustion starts late (CA5 3.2° BTDC). It is because more air mass is cooled down if methanol is

injected early leading to lower peak pressure. However, overall, Regarding the combustion phase, CA5 and ITE, all four test points shows similar results which suggest methanol injection timing has little effects on the combustion.

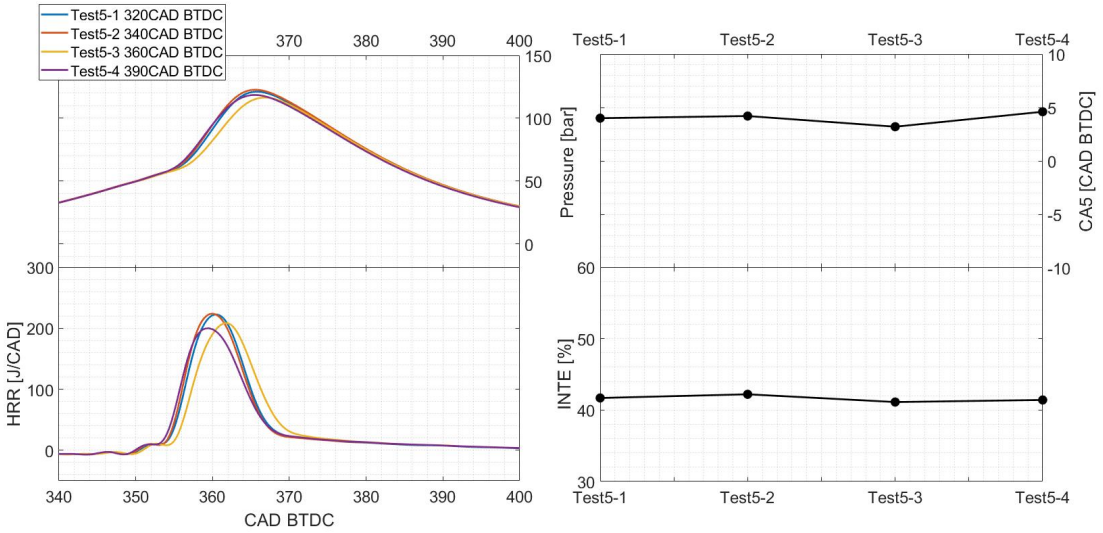


Figure 29: Effects of Methanol Injection Timing

4.3.2 Case 6: Effects of Air Intake Temperature

The fuel reactivity level is significantly enhanced by increasing the air intake temperature. Fig.30 compares the pressure and heat release curve of air intake temperature 20°C (Test6-1) and 25°C (Test6-2). When the air intake temperature is higher, the pressure rising is faster and advanced. The similar tendency is observed in heat release curve, that the HRR of Test6-2 is significantly rapid and early. Subsequently, the start of ignition is advanced from 2.8° BTDC in Test6-1 to 5° BTDC in Test6-2. Besides of CA5, the combustion duration of 25°C test is 1.2 CAD (0.133 ms) shorter than when the air intake temperature is 20°C. Due to the rapid combustion, CA50 of Test6-2 occurs at 1.4° BTDC which is not promising for engine operation. While the CA50 of Test6-1 occurs at -3.4° BTDC.

The temperature affects the fuel reactivity level from two aspects: increasing fuel evaporation rate and enhancing molecular movement which leads to a more homogeneous mixture. Therefore, when air intake temperature is 25°C, it is earlier to reach the auto-ignition point of premixed charge, and due to the better mixture of diesel and methanol, the transient procedure from diesel to methanol is faster.

The ITE of Test6-1 and Test6-2 is 42% and 44%, respectively. Although the peak of heat release happens before TDC in 25°C air intake test, which increases the negative power, it still has higher ITE than 20°C air intake test. The reason is in Test6-1, CA50 occurs so late that much less power is produced.

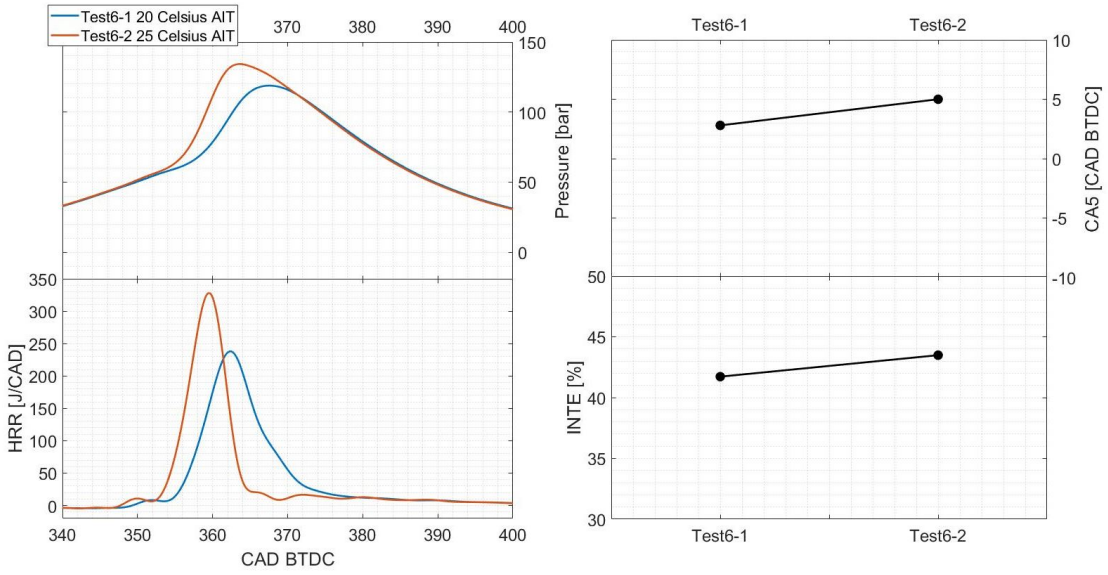


Figure 30: Effects of Air Intake Temperature

4.3.3 Case 7: Effects of Diesel Injection Timing for Different MSR

The diesel injection timing varies significantly in different MSR tests, but they share similar behaviours. To summarise, each MSR has a particular range of diesel SOI timing and the operation range is narrow. Fig.31 shows the pressure and heat release curve of 49% methanol substitution rate (Test7-2) where diesel is injected at 34, 34.5 and 35.5° BTDC. The optimal combustion occurs when diesel is delivered at 34.5° BTDC where the combustion starts at 4.2° BTDC, CA50 occurs at -1.0° BTDC and ITE is around 42%. When merely retarding diesel injection by 0.5 CAD, not only the combustion phase becomes advanced, but also the combustion is more rapid. In diesel SOI 34° BTDC case, the combustion begins at 4.6° BTDC and the CA50 occurs at TDC. Although the thermal efficiency is 0.5% higher than 34.5° BTDC diesel injection case, the heat release peak occurs too early to impair the engine. The diesel SOI 33.5° BTDC is also tested during the experiment, but the combustion is too aggressive that there is no time to record the pressure data. By contrast, when injecting diesel earlier by 1 CAD, the combustion phase is retarded, and most importantly, it becomes weak and unstable as the yellow curve shows in Fig.31. The peak pressure and peak heat release decrease significantly. The pressure curve fluctuation is observed during the experiment. Similarly, diesel SOI 36°

BTDC is also carried on, but the pressure rising is too inconspicuous to be detected.

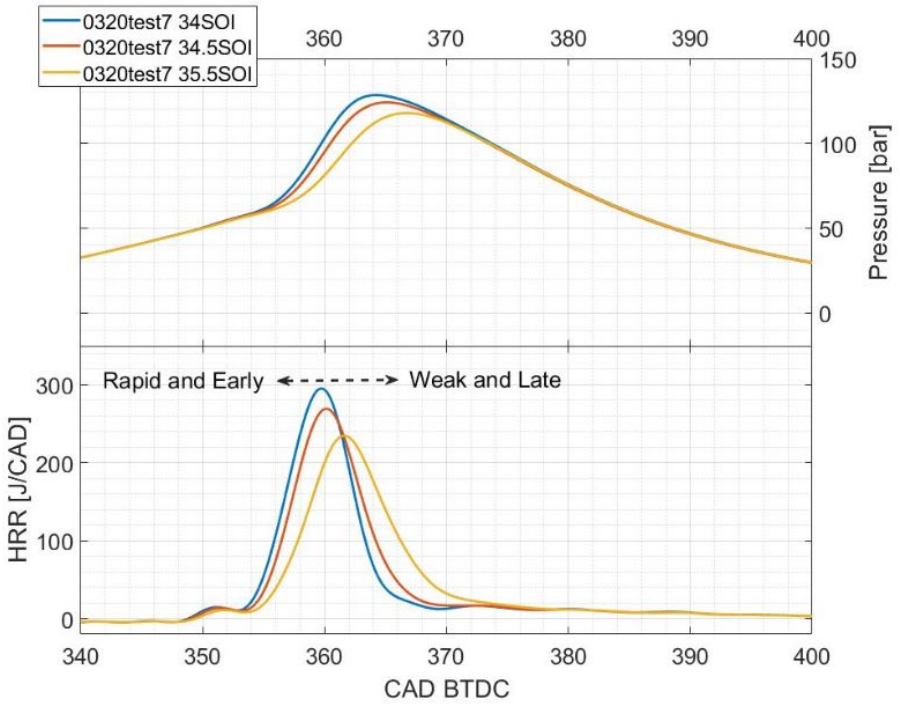


Figure 31: Pressure Rise and Heat Release of 49% MSR

The possible explanation for the phenomenon is the concentration of diesel. When diesel is injected late, the diesel fuel is dense in a specific region. The relatively concentrated diesel can be easier ignited when the in-cylinder temperature reaches the auto-ignition point and subsequently trigger the combustion of methanol. On the contrary, the early diesel injection makes diesel molecule sparse so that even if the in-cylinder has reached the diesel combustion conditions, the energy is still not enough to induce the diesel chemical reactions. It suggests early diesel injection requires richer air/fuel mixing conditions.

Similar tendency can also be seen in 37% (Test7-1), 58% (Test7-3), 62% (Test7-4) and 70% (Test7-5) MSR case. Fig.32 illustrates the pressure and heat release curve of them. As analysed before, in each methanol substitution rate, when injecting diesel late, the combustion becomes rapid and early, while if diesel is injected early, the combustion is weak and late. The maximum diesel SOI range is only 4 CAD.

It can be concluded from the phenomenon that no more than 4 CAD diesel SOI varies can decide the in-cylinder fuel mixing conditions which directly affect the methanol/diesel RCCI combustion. Besides, to stabilise the combustion, more air mass flow or lower air intake temperature can be used in late diesel SOI. While, in contrast, richer condition or higher air intake temperature is required when injecting

diesel early.

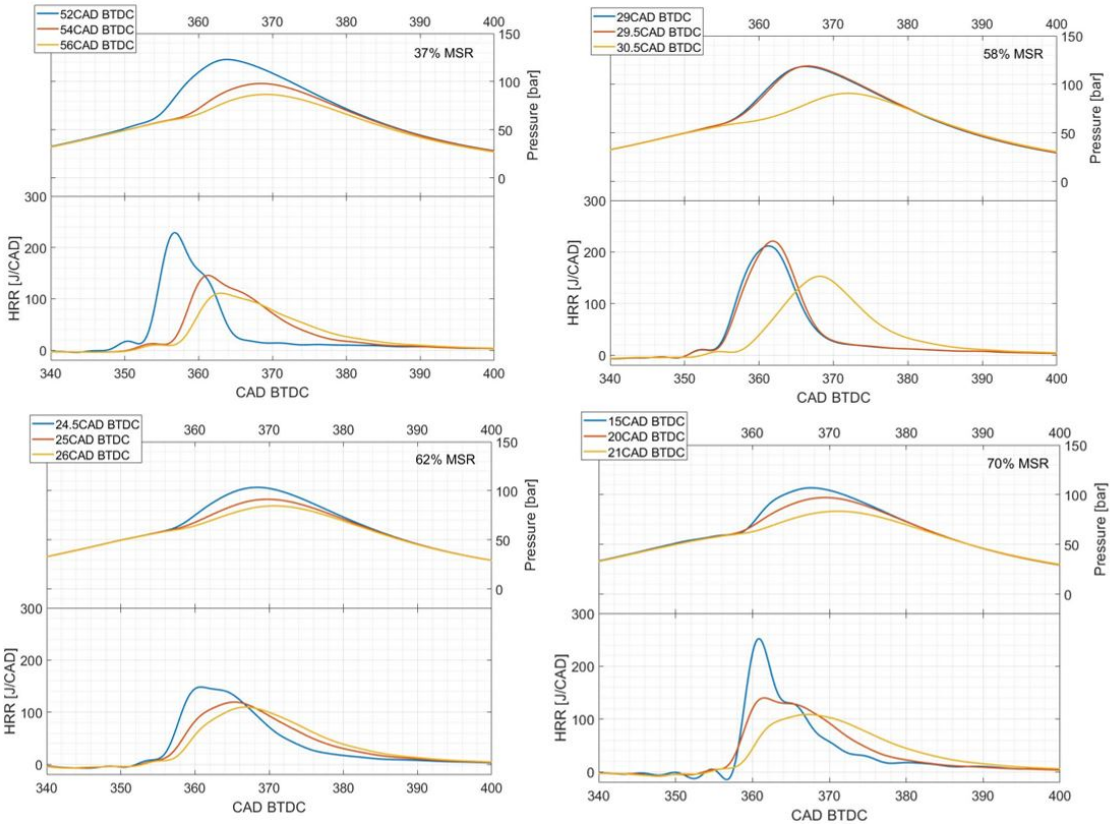


Figure 32: Effects of Diesel Injection Timing for Different MSR

Diesel SOI to methanol substitution rate is plotted in Fig.33. If comparing the diesel SOI at different methanol substitution rate, a linear tendency can be seen. When there is more diesel in the premixed charge, the appropriate diesel SOI timing is earlier (around 54° BTDC). If most energy is from diesel (37% MSR case), the combustion shows HCCI-like behaviours. On the one hand, if diesel is delivered a bit later when the in-cylinder temperature is high enough to ignite the diesel, the combustion will start too early. On the other hand, to control the combustion phase, the diesel should be injected at around 13° BTDC in which the combustion is dominant by dual fuel mechanism instead of RCCI. Thus, the diesel has to be injected early when the in-cylinder temperature is low so that the combustion will not start immediately.

However, if the methanol substitution rate is up to 70%, the promising diesel deliver timing is as late as 20° BTDC. The condition is opposite to the low MSR case. When the MSR is high, the overall fuel reactivity level is low. Therefore, early diesel injection will have ignition problems due to sparse diesel distribution. Late diesel injection can keep relatively high diesel cloud concentration to trigger the combustion reaction. The negative influence of high MSR is the methanol slip is high since

only 75% fuel is burned in this case.

By comparing the combustion of different methanol substitution rate, it can be summarised the MSR between 49% and 58% is the appropriate operation window. In this range, the methanol partial burning is lower, ITE is high, and the combustion phase is easier to control.

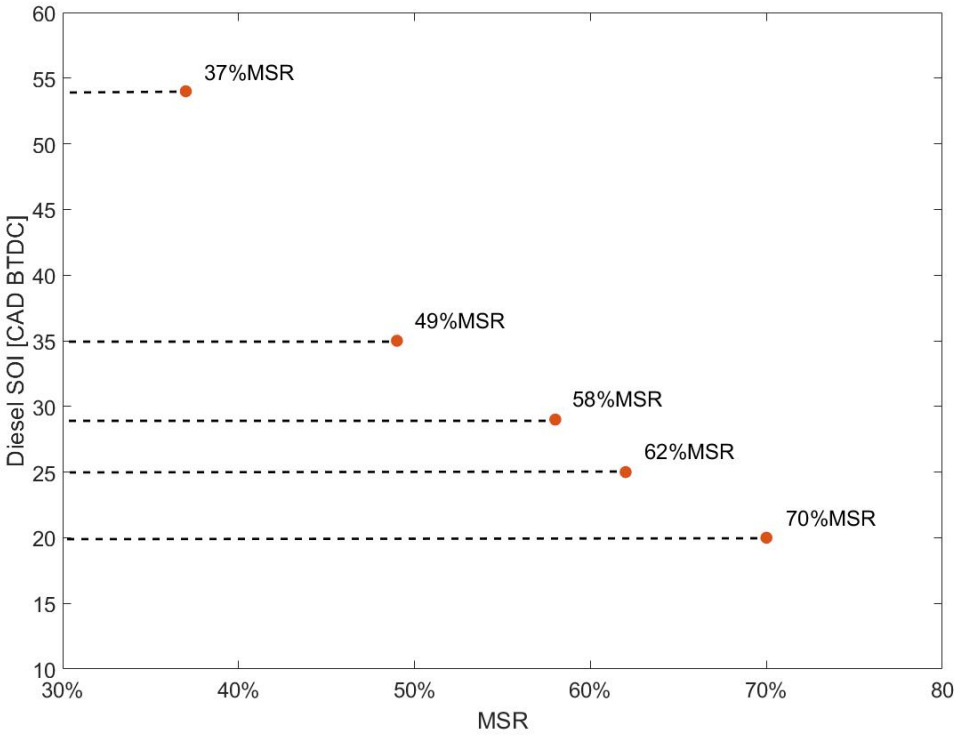


Figure 33: Corresponding Diesel Start of Injection Timing at Different Methanol Substitution Ratio

4.4 Results Summary

4.4.1 Combustion Characters Comparison

In order to understand combustion characters clearly, the pressure and heat release curves of a single diesel injection and a split diesel injection are compared directly. Both test points share the same air intake temperature(18°C), methanol injection timing(340° BTDC), total fuel energy content(2.89 kJ/cycle), MSR(56%) and ϕ(0.43). The only difference is that diesel is delivered once at 32° BTDC in single diesel injection test, but it is injected twice at 50° BTDC and 13° BTDC, respectively in split diesel case.

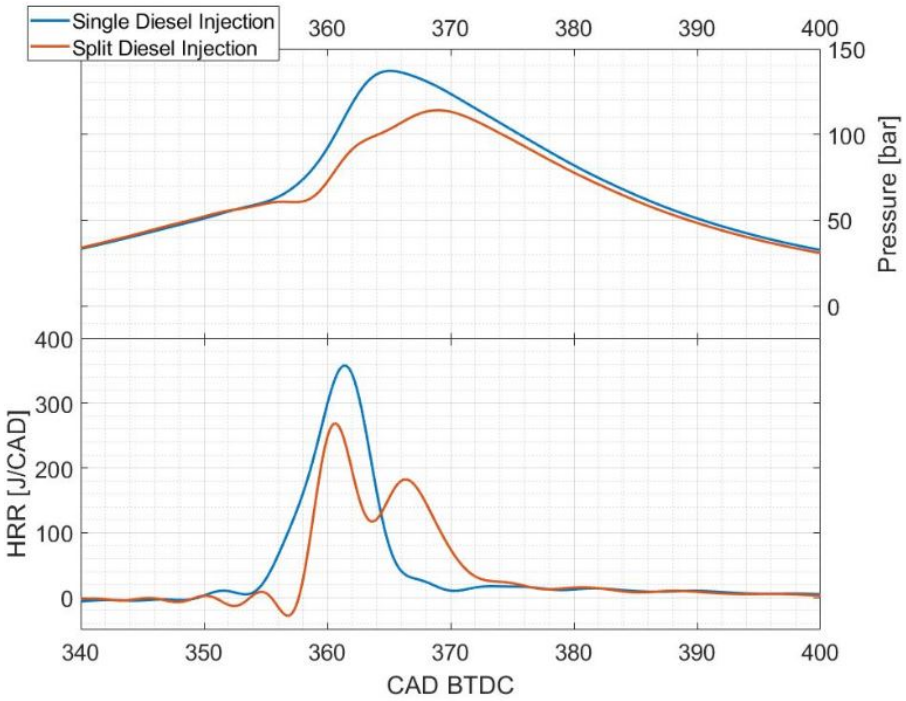


Figure 34: Heat Release Characters Comparison Between Single Diesel Injection and Split Diesel Injection

Two clear differences can be seen. First, the pressure rise of the single diesel injection experiment is uniform and smooth, but the pressure rise rate drops in the middle of combustion and then increases again in split diesel combustion case. Second, one main stage heat release (other than LTHR) can be seen in single diesel injection experiment, while two peaks occur in split diesel combustion.

The different HRR characters suggest the methanol/diesel RCCI combustion chemistry mechanism is significantly influenced by the diesel deliver strategy. In Single Diesel Injection test, as introduced in Section 4.3.1, the heat release starts from LTHR which subsequently leads to the combustion of premixed charge. By Contrast, in split diesel injection test, a rapid heat release is followed by a slower and longer heat release.

It can be observed that the HRR of single diesel injection test is slower than the first stage PRR of split diesel injection combustion. The phenomenon suggests the heat release of the single diesel injection test is from both methanol and diesel. The HRR is slowed down by the methanol component in the premixed charge. However, the first stage heat release of split diesel injection is only governed by diesel. Thus, HRR is faster in split diesel injection case.

The ITE of single diesel injection is 42% which is one percent higher than that of

split diesel injection. The reason is the fuel burning rate in the single diesel injection case is around 87% while only 83% fuel is burned in the split diesel case. As a result, more power is produced in the single diesel case. Ultimately, the diesel and methanol have better mixing conditions when diesel is injected once, so the combustion rate is fast to burn more fuel. In this scenario, the combustion is not governed by the flame propagation, since diesel particles in the premixed charge result in homogeneous ignition at different locations simultaneously. However, when diesel is injected twice, there is pilot diesel diffusion flame and premixed flame propagation, but it is not fast to burn all the methanol leading to more methanol partial burning.

4.4.2 Combustion Temperature and NOx Emissions

Fig.35 compares NOx emissions of Test6-1 in which the air intake temperature is 20°C and Test6-2 in which air intake temperature is 25°C. As it can be seen, only five degrees of temperature rising almost doubles the NOx emissions.

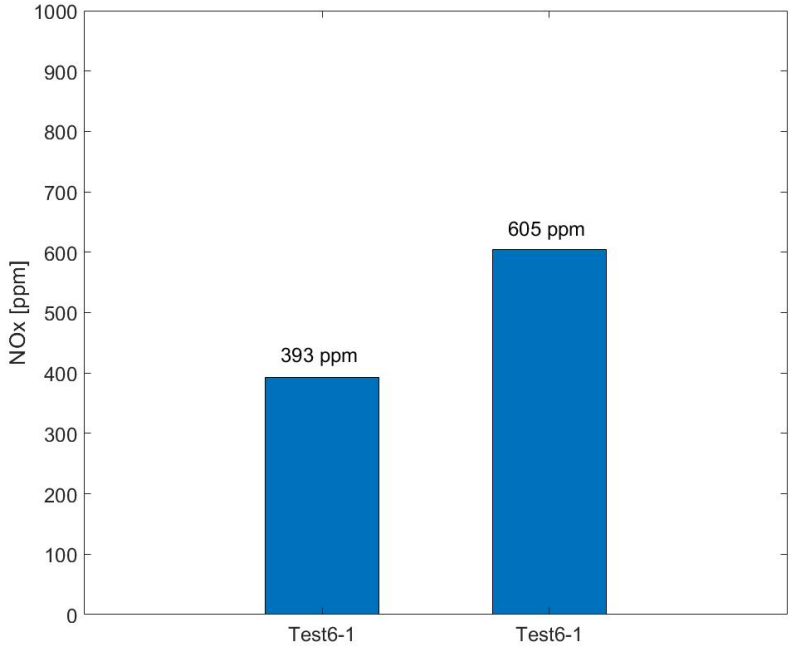


Figure 35: NOx Emissions Comparison of Different Air Intake Temperature. Test6-1: 20°C Air Intake; Test6-2: 25°C

The experiment results also indicate the NOx emission behaviours are highly dependent on diesel injection strategies. Fig.36 compares the NOx emissions of single diesel injection (Test5-1 to Test5-4) and split diesel injection (Test1-1 to Test1-3). The air intake temperature(18°C), MSR(54%) and total fuel energy(2.89 kJ/cycle) are the same.

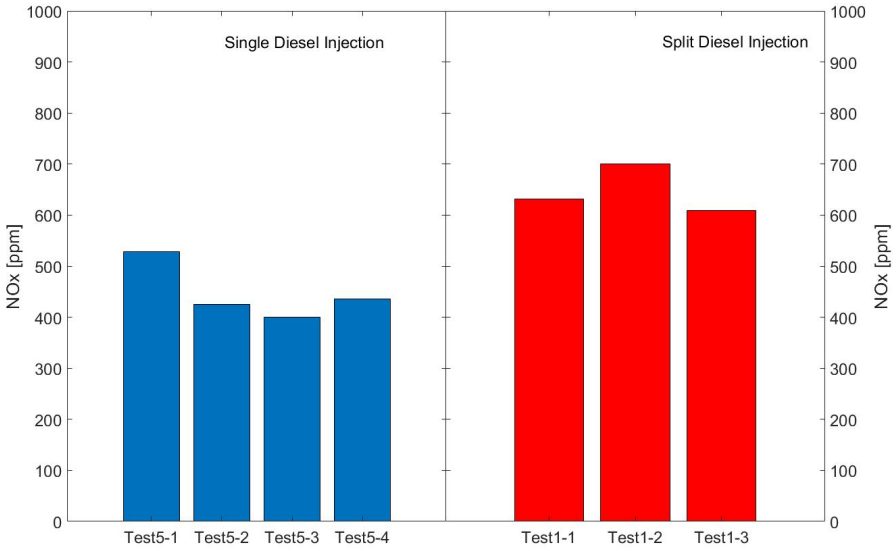


Figure 36: NOx Emission Comparison of Single Diesel Injection and Split Diesel Injection

It shows that the NOx emission in split diesel injection is around 150 ppm higher than the data of single diesel injection. The main reason for the different NOx emissions is the combustion character. In split diesel injection case, the combustion is similar to diesel combustion or dual fuel combustion. The pilot diesel injection leads to diesel jet combustion and diffusion flames which results in NOx formation in the fuel rich region. However, in the single diesel injection experiment, there is no local diesel rich zone due to pre-injected diesel. Thus, the high temperature rich fuel zone is avoided.

4.4.3 Fuel Reactivity

Reactivity refers to the rate that reactants tend to undertake chemical reactions. Specifically, in the internal combustion engine, it refers to the rate of fuel oxidation. The main idea of RCCI combustion is to use methanol to reduce the reactivity level of diesel HCCI combustion. If the in-cylinder methanol, diesel and air mix ideally even, the combustion rate can be slowed down. Theoretically, if the in-cylinder charge is mixed homogeneously, which is mainly dependent on diesel injection strategy, the fuel reactivity relies on ϕ, methanol substitution rate and air intake temperature. At this moment, the fuel reactivity level can be summarised based on experiment results, and there are mainly two categories based on diesel injection strategy.

In the first scenario, the diesel and methanol are not well mixed, which mainly refers to split diesel injection cases. The premixed diesel has abundant time to mix with methanol, but the pilot diesel injection creates a local high reactivity zone. This

diesel rich zone results in diesel combustion and diffusion flame propagation. The methanol reactivity control is mainly reflected in the premixed charge combustion stage where there is premixed flame propagation. The premixed diesel is delivered very early so that diesel and methanol can be regarded as homogeneous mixing. Thus, there is a clear reactivity stratification in the split diesel case: the high reactivity diesel pilot zone and reactivity controlled premixed region. As shown in the experiment results, the combustion is dominated by the pilot diesel injection because the split diesel RCCI shows dual fuel or diesel combustion characters including high NOx and high combustion temperature.

In the second scenario, the mixing condition of diesel and methanol can be assumed homogeneously, which is represented by single diesel injection cases. According to *Case 6: Study of Air Intake Temperature*, the RCCI fuel reactivity is directly affected by the charge air temperature. It is because the high temperature increases the fuel internal energy so that the fuel is more accessible to be ignited. Besides, high methanol substitution rate reduces the fuel reactivity. It is supported by the experiment phenomenon that the methanol incomplete burning is significant in high MSR case. For example, in Test7-4 and Test7-5 that have higher than 60% MSR, considerable methanol partial burning is observed. However, the experiment does not reach the ideal methanol/diesel mixing condition since the diesel cloud concentration has the influence on the combustion. As analysed in Section 4.3.3, the diesel SOI timing affects the diesel fuel distribution in the premixed charge which further influences the combustion.

5 Conclusions

The thesis systematically studied the RCCI combustion principles and reviewed the previous works. Based on the literature study, the critical parameters of methanol/diesel RCCI combustion has been identified, and the experiment has tested a wide range of variables. Combustion characteristics are analysed via the recorded pressure curve and heat release curve.

Theoretically, RCCI combustion requires diesel and methanol to mix homogeneously, but in practical, the ideal homogeneous mixture condition is tough to reach. The combustion starts with diesel particles which further ignite methanol. Most of the current RCCI researches inject diesel earlier than 15° BTDC to reach RCCI like combustion, and in order to stabilise the combustion, diesel injection is always split. However, researchers have different understanding to RCCI technology due to insufficient research, and thus, many RCCI combustion researches show either dual fuel like behaviours or the combustion starts too early for engines. In this master thesis, to achieve the study objective, the experiment attempts to measure air mass flow, air intake temperature, methanol substitution rate, methanol injection timing and diesel injection strategy. The master thesis tries to investigate how to reach the theoretical RCCI combustion, the experiments results are presented in Chapter 4 and the key points are concluded in the following paragraphs.

The combustion mechanism is the fundamental factor to distinguish RCCI combustion and dual fuel combustion. To reach the RCCI combustion zone, the air intake temperature is required to be high. As the results of GT-SUITE simulation suggest, air intake temperature greater than 40°C is necessary to diminish the effects of methanol evaporation. A research conducted in King Abdullah University of Science and Technology even used 200°C air intake temperature. Additionally, it is illustrated by the experiment that the methanol/diesel RCCI combustion can be divided into two groups according to the combustion behaviour. Practically, the diesel injection strategy has a great influence on the combustion mechanism, because it decides the fuel reactivity stratification. Accordingly, the thesis experiment can be divided into two groups: (1) Split diesel injection experiment where it has dual fuel combustion behaviours. The combustion starts from pilot diesel ignition followed by pilot diesel diffusion flame propagation and premixed end gas combustion; (2) Single diesel injection that results in RCCI combustion. The diesel diffusion flame does not occur and the combustion starts from LTHR which is followed by simultaneous combustion of the premixed charge. Other than the combustion character, the influence of parameters in each group can be summarised:

(1) Split diesel injection

- Methanol injection timing does not have significant influences on the methanol/diesel combustion concerning combustion phase, ITE and NOx emissions.
- Air mass flow affects premixed flame propagation directly. There is no com-

plete premixed flame propagation observed in rich conditions when the equivalent ratio is lower than 0.42 (Air mass flow 80 kg/h and 90 kg/h).

- Air intake temperature strongly actives the combustion. 70°C air intake temperature leads to early, rapid combustion and single stage heat release.
- Methanol substitution rate is discovered in middle load (IMEP: 7.5 bar) and high load (IMEP: 12 bar). Premixed flame propagation has taken place in high load case, since two heat release peak occurs. While there is no explicit premixed flame propagation in middle load conditions, especially when MSR is lower than 56%. Besides, it is observed combustion is retarded with MSR increasing.

(2) Single diesel injection

- Methanol injection timing of the single diesel injection experiment has similar behaviour as split diesel case that it does not affect the combustion significantly.
- Air intake temperature strongly actives the combustion. Increasing air intake temperature from 20°C to 25°C, the CA50 advanced from -3.5° BTDC to 0.2° BTDC.
- Methanol substitution rate has great influence on the RCCI combustion and it decides diesel SOI timing directly. For a particular MSR, there is a certain and narrow diesel SOI range. Besides, if MSR is lower than 30%, the combustion is hard to control and the advantages of RCCI cannot be seen. While if MSR higher than 70%, the partial combustion is significant. Thus, the optimal MSR used in the experiment is between 47% to 58%.

To summarise, the optimal conditions to operate methanol/diesel fuel in RCCI condition is 45% to 60% MSR, 30°C to 50°C air intake temperature and around 35° BTDC diesel injection timing.

6 Future Work

In order to reach theoretical RCCI combustion conditions, single diesel injection strategy or split diesel injection with delivering pilot diesel earlier than 15° BTDC should be conducted.

Upon this injection strategy, at a certain methanol substitution rate, there are two aspects of studying the equivalent ratio: the bottom limit in lean conditions of misfire and up limit in rich conditions of diesel components early combustion. Misfire can be prevented by increasing the air intake temperature, but high air intake temperature will result in premixed fuel early combustion. To balance the influence of air intake temperature, it is necessary to investigate the impact of EGR. Additionally, the thesis has concluded the MSR higher than 70% will lead to incomplete burning, but the experiment was conducted at ambient air intake conditions. With higher charge air temperature, the upper limit of MSR should be discovered. Similarly, EGR would be needed to control the combustion.

Additionally, Prof. Bengt Johansson from King Abdullah University of Science and Technology recommended that the methanol/diesel RCCI combustion should start from pure methanol HCCI mode with more than 150°C air intake temperature. After methanol HCCI combustion has been reached, inject a little amount of diesel and meanwhile reduce air intake temperature. This valuable recommendation also provides a new strategy for future RCCI operation.

References

[1] World: Balance for 2015. *International Energy Agency,* http://www.cs.uku.fi/~kilpelai/wwwlahteet.html.

[2] Volvo bioDME – CO_2 neutral transport in reality. *Volvo group,* https://www.aboutdme.org/aboutdme/files/ccLibraryFiles/Filename/000000002392/BioDME_Volvo_brochure.pdf.

[3] Thring, R. Homogeneous charge compression ignition (HCCI) Engines. *SAE Technical Paper, 892068,* 1989.

[4] Reitz, R., Duraisamy, G. Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines. *Progress in Energy and Combustion Science,* 2014.

[5] Methanol. *PubChem, U.S. National Library of Medicine,* 2018 https://pubchem.ncbi.nlm.nih.gov/compound/methanol#section=Top.

[6] Methanol Industry. *Methanol Institute,* http://www.methanol.org/the-methanol-industry/.

[7] Methanol Production. *Marine Methanol,* http://marinemethanol.com/about-methanol/methanol-production.

[8] Aasberg, K., Nielsen, C. Large scale methanol production from natural gas. *Haldor Topsoe,* 2008, vol. 22.

[9] Demirbas, A. Biodiesel production from vegetable oils via catalytic and non-catalytic supercritical methanol transesterification methods. *Progress in Energy and Combustion Science,* 2005, vol. 31, Issue 5-6, 466-487.

[10] Automotive fuels - Diesel - Requirements and test methods. *EUROPEAN STANDARD,* April 2009. http://www.envirochem.hu/www.envirochem.hu/documents/EN_590_2009_hhV05.pdf.

[11] Automotive fuels - Unleaded petrol - Requirements and test methods. *EUROPEAN STANDARD,* July 2008. http://www.envirochem.hu/www.envirochem.hu/documents/EN_228_benzin_JBg37.pdf.

[12] Ethanol. *PubChem, U.S. National Library of Medicine,* 2018 https://pubchem.ncbi.nlm.nih.gov/compound/ethanol.

[13] Tuominen, T. Potential of Methanol in Dual Fuel Combustion. *Aalto University Master Thesis,* Espoo, 2016.

[14] Diesel and gasoline. *Advanced Motor Fuels.* http://www.iea-amf.org/content/fuel_information/diesel_gasoline#diesel.

[15] Basshuysen, R, Schäfer, F. Internal Combustion Engine Handbook *SAE International,* 2004. Wiesbaden, Germany. ISBN: 0-7680-1139-6

[16] Song, J., Kraipat, C., Wang, J. Effect of Oxygenated Fuel on Combustion and Emissions in a Light-Duty Turbo Diesel Engine. *Energy & fuels,* 2002, 16(2), pp 294-301.

[17] Next generation of methanol fuel cell vehicles sees the light of day. *Serenergy,* `https://serenergy.com/next-generation-of-methanol-fuel-cell-vehicles-sees-the-light-of-day/` .

[18] Tuner, M., Aakko-Saksa, P., Molander, P. Engine Technology, Research, and Development for Methanol in Internal Combustion Engines. *SUMMETH-Sustainable Marine Methanol,* 2018-03-26.

[19] Andersson, K., Salazar, C.M. METHANOL AS A MARINE FUEL REPORT. *FCBI energy,* 2015.

[20] Using Methanol Fuel in the MAN B&W ME-LGI Series *MAN Diesel & Turbo*

[21] Heywood, J. Internal Combustion Engine Fundamentals *McGRAW-HILL,* 1998. New York, NY. ISBN: 0-07-100499-8

[22] Pettinen, R. Dual-fuel combustion characterzation on lean conditions and high loads. *Aalto University Master Thesis,* Espoo, 2016.

[23] Dec, J. A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet imaging. *SAE Technical Paper,* 1997-02-24-970873.

[24] Karim, G. A. Combustion in Gas Fueled Compression: ignition Engines of the Dual Fuel Type. *Journal of Engineering for Gas Turbines and Power,* July 2003, Vol. 125.

[25] Ahmad, Z., Aryal, J., Ranta, O., et al. An Optical Characterisation of Dual-Fuel Combustion in a Heavy-Duty Diesel Engine. *SAE Technical Paper,* 2018-01-0252.

[26] Stanglmaier, R., Roberts, C. Homogeneous Charge Compression Ignitino (HCCI): Benefits, Compromises and Future Engine Applications. *SAE Technical Paper,* Toronto, Ontario, Canada. 1999-01-3682.

[27] Yao, M., Zheng, Z., Liu, H. Progress and recent trends in homogeneous charge compression ignition (HCCI) engines. *Progress in Energy and Combustion Science,* 35(2009) 398-437

[28] Helmantel, A., Ingemar, D. HCCI Operation of a Passenger Car Common Rail DI Diesel Engine with Early Injection of Conventional Diesel Fuel. *SAE Technical Paper,* 2004-01-0935.

[29] Jia, Z.Q., Denbratt, I. Experimental investigation into the combustion characteristics of a methanol-Diesel heavy duty engine operated in RCCI mode. *Fuel,* Aug 2018, Vol. 226, Pages 745-753.

[30] Inagaki, k., et al. Dual-Fuel PCI Combustion Controlled by In-Cylinder Stratification of Ignitability. *SAE Technical Paper,* 2004-01-0935.

[31] Li, J., Yang, W., Zhou, D. Review on the management of RCCI engines. *Renewable and Sustaibale Energy Reviews,* 2017.

[32] Li, Y., Jia, M., Liu, Y., Xie, M. Numerical study on the combustion and emission characteristics of a methanol/diesel reactivity controlled compression ignition (RCCI) engine. *Applied Energy,* 2013.

[33] Kokjohn, S., Reitz, R., Splitter, D. Investigation of Fuel Reactivity Stratification for Controlling PCI Heat-Release Rates using High-Speed Chemiluminescence Imaging and Fuel Tracer Fluorescence. *SAE International Journal of Engines,* 2012-01-0375.

[34] Splitter, D., Hanson, R., Kokjohn, S., et al. Injection Effects in Low Load RCCI Dual-Fuel Combustion *SAE International Journal of Engines,* 2011-24-0047.

[35] Li, Y., Jia, M., et al. Parametric study and optimisation of a RCCI (reactivity controlled compression ignition) engine fueled with methanol and diesel *Energy,* 2013.

[36] Li, Y., Jia, M., et al. Evaluation of the necessity of exhaust gas recirculation employment for a methanol/diesel reactivity controlled compression ignition engine operated at medium loads *Energy Conversion and Management,* 2015.

[37] Blumberg, P. Simulation of a Boosted, Dual-fuel 'octane-on-demand' PFI/DI Engine for the Purpose of Knock Prediction *GT-SUITE Users Conference,* Frankfurt, 2015.

[38] Eng, J.A. Characterization of Pressure Waves in HCCI Combustion *SAE Technical paper,* 2002-01-2859.

[39] Zhou, D.Z., Yang, W.M., et al. Application of CFD-chemical kinetics approach in detecting RCCI engine knocking fuelled with biodiesel/methanol *Applied Energy,* 2015.

[40] Li, Y.P., Jia, M., et al. Towards a comprehensive understanding of the influence of fuel properties on the combustion characteristics of a RCCI (reactivity controlled compression ignition) engine *Energy,* 2016.

[41] Prabhakar, B., Jayaraman, S., et al. Experimental Studies of High Efficiency Combustion With Fumigation of Dimethyl Ether and Propane Into Diesel Engine Intake Air *Journal of Engineering for Gas Turbines and Power,* Apr. 2015.